```
=> d que
L1                STR

                   25  41
 CH~Ak             O   G4
@39 40             ‖   ‖
                G3~C~~C~C~G2
                21  22  23  24

VAR G2=H/ME
VAR G3=ME/ET
VAR G4=CH2/39
NODE ATTRIBUTES:
CONNECT IS E1  RC AT  40
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   8

STEREO ATTRIBUTES: NONE
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                 ELC.SUB=3 NOT (PMS OR IDS)/CI
L4           681 SEA FILE=REGISTRY SUB=L2 SSS FUL L1
L5          1237 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L4(L)PREP/RL
L17              TRANSFER  PLU=ON  L5 1- RN :   22032 TERMS
L18        22026 SEA FILE=REGISTRY ABB=ON  PLU=ON  L17
L19          487 SEA FILE=REGISTRY ABB=ON  PLU=ON  L18 AND (ZR OR TI OR HF)/ELS

L22              STR

O≡C~C
1  2  3


NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   3

STEREO ATTRIBUTES: NONE
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L25              STR

CH=O
1  2


NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   2
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STEREO ATTRIBUTES: NONE
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L28 318944 SEA FILE=HCAPLUS ABB=ON PLU=ON L24(L)(RACT OR RCT OR RGT)/RL

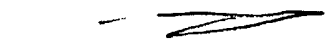
L29 136231 SEA FILE=HCAPLUS ABB=ON PLU=ON L26(L)(RACT OR RCT OR RGT)/RL

L30 470 SEA FILE=HCAPLUS ABB=ON PLU=ON L5 AND L28 AND L29
L32 12 SEA FILE=HCAPLUS ABB=ON PLU=ON L30 AND L19(L)CAT/RL

no gem-dimethyl rings in this set.

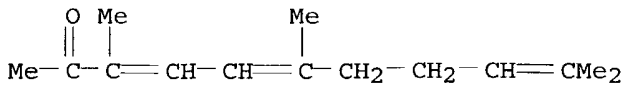
=>d l32 ibib ab hitind hitstr 1-12

L32 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:939536 HCAPLUS
DOCUMENT NUMBER: 140:271020
TITLE: Synthesis of isomethyl-ionone
AUTHOR(S): Huang, Xi-gen; Zhao, Ai-jun; Xi, Yun-qun; Huang, Shuang-gen; Liu, Xiao-geng
CORPORATE SOURCE: Institute of Applied Chemistry, Jiangxi Agricultural University, Nanchang, Jiangxi, 330045, Peop. Rep. China
SOURCE: Jingxi Huagong (2003), 20(10), 605-608
CODEN: JIHUFJ; ISSN: 1003-5214
PUBLISHER: Jingxi Huagong Bianjibu
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
OTHER SOURCE(S): CASREACT 140:271020
AB A new method for synthesis of methyl-ionones by cyclization reaction of pseudo-isomethyl-ionone catalyzed by solid supported strong acid-TiO2/SO42-. The optimum conditions were n(pseudo-isomethyl-ionone):n(xylene):n(sulfuric acid) = 1:3.5:0.05, reaction temperature 15-25 °C and reaction time 1.5 h. Under the optimum conditions the yield was 92% -93% with the content of α-isomethyl-ionone 77%.
CC 30-15 (Terpenes and Terpenoids)
IT **13463-67-7**, Titanium dioxide, uses 14808-79-8, Sulfate, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(as solid supported acid)
IT **1117-41-5P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; **RACT (Reactant or reagent)**
(as solid supported acid)
IT **78-93-3**, 2-Butanone, reactions **5392-40-5**, Citral
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(synthesis of isomethylionone via solid supported strong acid)
IT **13463-67-7**, Titanium dioxide, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(as solid supported acid)
RN 13463-67-7 HCAPLUS
CN Titanium oxide (TiO2) (8CI, 9CI) (CA INDEX NAME)

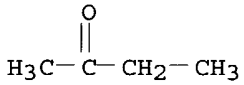


IT **1117-41-5P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; **RACT (Reactant or reagent)**
(as solid supported acid)
RN 1117-41-5 HCAPLUS

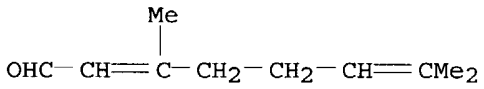
CN 3,5,9-Undecatrien-2-one, 3,6,10-trimethyl- (8CI, 9CI) (CA INDEX NAME)



IT **78-93-3**, 2-Butanone, reactions **5392-40-5**, Citral
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(synthesis of isomethylionone via solid supported strong acid)
RN 78-93-3 HCAPLUS
CN 2-Butanone (8CI, 9CI) (CA INDEX NAME)



RN 5392-40-5 HCAPLUS
CN 2,6-Octadienal, 3,7-dimethyl- (8CI, 9CI) (CA INDEX NAME)



L32 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:454193 HCAPLUS
DOCUMENT NUMBER: 139:36650
TITLE: Device and method for carrying out heterogeneously-catalyzed reactive distillations in particular for the production of pseudoionone
INVENTOR(S): Kaibel, Gerd; Miller, Christian; Dobler, Walter; Dirnsteiner, Thomas; Sigl, Marcus; Jansen, Helmut; Kaibel, Bjoern
PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 30 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003047747	A1	20030612	WO 2002-EP13796	20021205

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,

PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

DE 10159821 A1 20030618 DE 2001-10159821 20011206

PRIORITY APPLN. INFO.: DE 2001-10159821 A 20011206

OTHER SOURCE(S): CASREACT 139:36650

AB The invention relates to a column for carrying out reactive distns. in the presence of a heterogeneous particulate catalyst, with a packing or filling bodies, which form cavities in the column interior. The quotient for the hydraulic diameter for the gas stream through the packing or filling bodies and the equivalent diameter of the catalyst particles lies in the range of 2 to 20, preferably in the range of 5 to 10, whereby the catalyst particles are introduced loose into the cavities, distributed and removed under the influence of gravity (schematics included). Thus, citral and acetone are pumped into a distillation column containing praseodymium on γ-Al2O3 heated to 124°; the condensate contains 66.7% pseudoionone (based on citral).

IC ICM B01J019-32
ICS B01J008-00; B01J023-10; B01J008-02; C07C045-28; B01D003-00

CC 30-10 (Terpenes and Terpenoids)
Section cross-reference(s): 48

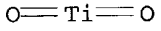
IT 1344-28-1, Alumina, uses 7440-10-0D, Praseodymium, catalysts
13463-67-7, Titanium dioxide, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(heterogeneously-catalyzed reactive distns. in particular for the production of pseudoionone)

IT **67-64-1**, Acetone, reactions **5392-40-5**, Citral
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(heterogeneously-catalyzed reactive distns. in particular for the production of pseudoionone)

IT **141-10-6P**, Pseudoionone
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(heterogeneously-catalyzed reactive distns. in particular for the production of pseudoionone)

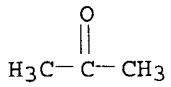
IT **13463-67-7**, Titanium dioxide, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(heterogeneously-catalyzed reactive distns. in particular for the production of pseudoionone)

RN 13463-67-7 HCAPLUS
CN Titanium oxide (TiO2) (8CI, 9CI) (CA INDEX NAME)



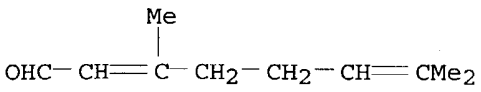
IT **67-64-1**, Acetone, reactions **5392-40-5**, Citral
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(heterogeneously-catalyzed reactive distns. in particular for the production of pseudoionone)

RN 67-64-1 HCAPLUS
CN 2-Propanone (9CI) (CA INDEX NAME)

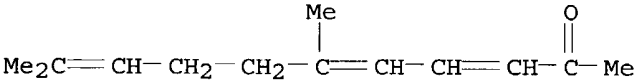


RN 5392-40-5 HCAPLUS

CN 2,6-Octadienal, 3,7-dimethyl- (8CI, 9CI) (CA INDEX NAME)



IT **141-10-6P**, Pseudoionone
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(heterogeneously-catalyzed reactive distns. in particular for the production of pseudoionone)
RN 141-10-6 HCAPLUS
CN 3,5,9-Undecatrien-2-one, 6,10-dimethyl- (8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:25147 HCAPLUS
DOCUMENT NUMBER: 140:146179
TITLE: Product class 11: organometallic complexes of zirconium and hafnium
AUTHOR(S): Negishi, E.-I.; Takahashi, T.
CORPORATE SOURCE: Department of Chemistry, Purdue University, West Lafayette, IN, 47907, USA
SOURCE: Science of Synthesis (2003), 2, 681-848
CODEN: SSCYJ9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review of application and preparation of organometallic complexes of zirconium and hafnium.
CC 29-0 (Organometallic and Organometalloidal Compounds)
IT **84987-26-8**
RL: **CAT (Catalyst use)**; RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(review of application and preparation of organometallic complexes of zirconium and hafnium)
IT **7440-58-6DP**, Hafnium, organometallic complexes **7440-67-7DP**, Zirconium, organometallic complexes
RL: **CAT (Catalyst use)**; RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(review of application and preparation of organometallic complexes of zirconium and hafnium)
IT **148276-57-7P 148347-89-1P 148347-91-5P 148347-92-6P**
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(review of application and preparation of organometallic complexes of zirconium and hafnium)
IT 75-64-9, reactions 87-62-7 87-85-4 90-15-3, 1-Naphthalenol **93-53-8** 95-93-2 96-10-6, reactions 97-93-8, reactions

98-88-4, Benzoyl chloride 100-42-5, reactions 100-99-2, reactions
103-30-0 **104-53-0**, Benzenepropanal 106-95-6, reactions
108-88-3, reactions 109-06-8 109-64-8 109-74-0, Butanenitrile
109-96-6 110-57-6 110-87-2 111-66-0, 1-Octene 115-07-1, 1-Propene,
reactions 115-11-7, reactions **123-38-6**, Propanal, reactions
124-13-0, Octanal 300-57-2 501-65-5 **502-56-7**,
5-Nonanone 503-17-3, 2-Butyne 503-60-6 513-35-9 530-93-8
536-74-3 538-75-0 544-25-2, 1,3,5-Cycloheptatriene 557-20-0
557-40-4 563-79-1 588-59-0 589-09-3 590-18-1 591-50-4
592-41-6, 1-Hexene, reactions 592-42-7, 1,5-Hexadiene 593-60-2
615-42-9 **617-35-6** 624-64-6 627-21-4, 2-Pentyne 629-05-0,
1-Octyne 629-20-9, 1,3,5,7-Cyclooctatetraene 636-31-7 644-97-3
672-66-2 682-00-8 691-37-2 695-12-5 696-28-6 764-35-2, 2-Hexyne
764-93-2, 1-Decyne 769-92-6 775-12-2 872-05-9, 1-Decene 927-74-2,
3-Butyn-1-ol 927-80-0 928-49-4, 3-Hexyne 930-68-7,
2-Cyclohexen-1-one 930-81-4 999-78-0 1109-15-5 1291-32-3
1461-22-9 1476-11-5 1708-29-8 1708-32-3 1823-14-9 1849-28-1
1942-45-6, 4-Octyne 1942-46-7, 5-Decyne 2123-72-0 2170-08-3
2622-21-1 2678-95-7 2769-64-4 2787-43-1 2789-89-1 3017-70-7
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1,7-Octadiene 3839-31-4 4045-44-7 4210-32-6 4440-01-1 4805-17-8
4984-82-1 5172-02-1 5296-64-0 5666-17-1 **6213-87-2**
6224-91-5 6699-93-0 6833-44-9 7188-38-7 10060-17-0 10568-44-2
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13667-12-4 13846-40-7 14543-49-8 14630-40-1 16133-78-1
16387-70-5, 3,5-Octadiyne 16644-98-7 19756-04-8 21020-27-9
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21959-01-3 21959-05-7 22433-33-6, 1,2-Nonadiene 23377-91-5
23578-51-0, 2,7-Octadien-1-ol 23708-47-6 23978-09-8 24356-01-2
24544-04-5 24774-58-1 25015-63-8 25017-02-1 29765-03-5
31600-86-9 33100-27-5, 1,4,7,10,13-Pentaoxacyclopentadecane 34034-67-8
34721-46-5, 7,8-Dicarbaundecaborane(13) 36942-56-0 37206-41-0
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39768-05-3 41417-50-9 41823-71-6 42423-66-5 **50396-96-8**
51177-89-0 51231-81-3 51391-25-4 53877-58-0 54634-14-9
54634-15-0 54813-19-3 55718-76-8 56592-41-7 59936-29-7
60938-62-7 61160-65-4 61396-34-7 62263-69-8 63175-87-1
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80005-42-1 80789-51-1 81476-64-4 82135-42-0 84278-90-0
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116436-94-3 117897-78-6 118573-45-8 119594-68-2 120059-92-9
120989-99-3 121918-58-9 122445-21-0 123858-02-6 124244-39-9
124380-41-2 125843-99-4 128923-40-0 130031-73-1
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(review of application and preparation of organometallic complexes of zirconium and hafnium)

IT 130031-74-2 132514-22-8 133896-92-1 135469-08-8 135610-09-2
135760-86-0 137594-89-9 139129-16-1 142021-37-2 143212-50-4
144777-55-9 146330-82-7 147659-31-2 148200-41-3 148200-42-4
148420-63-7 148751-69-3 150344-92-6 150584-28-4, 2,7-Dodecadiyne
150615-36-4 151138-08-8 151138-09-9 151459-69-7 152253-16-2

155167-77-4 155835-37-3 157835-98-8
157948-80-6 158676-45-0 158676-46-1 158700-34-6 159531-47-2
160298-02-2 160929-09-9 162053-09-0 163086-42-8 163591-69-3
164662-87-7 166279-55-6 166825-50-9 166988-06-3 166988-07-4
170504-16-2 177327-38-7 180866-31-3 181823-43-8 184033-98-5
184704-18-5 186002-85-7 186002-86-8 186891-73-6 188297-24-7
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211799-38-1 223506-82-9 243870-18-0 243870-26-0 253202-93-6
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651299-70-6 651300-00-4 651300-32-2 651300-33-3 651300-34-4
651300-37-7 651300-38-8 651300-41-3 651300-49-1 651300-50-4
651300-51-5
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(review of application and preparation of organometallic complexes of zirconium and hafnium)

IT 529-34-0P 558-37-2P 1291-45-8P 1298-41-5P 2171-98-4P 12097-04-0P
12116-66-4P 34767-44-7P 39292-59-6P 39292-60-9P 50648-05-0P
53433-58-2P 54039-38-2P 61396-31-4P 67659-93-2P 70302-43-1P
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113035-23-7P 118141-77-8P 118141-78-9P 118141-79-0P 118141-80-3P
122445-16-3P 122445-20-9P 125843-96-1P 129174-25-0P 132100-78-8P
132100-79-9P 133817-48-8P 147659-30-1P **157836-00-5P**
159540-08-6P 159574-30-8P 163090-91-3P **180866-33-5P**
201658-51-7P 201658-59-5P 259129-36-7P 651300-16-2P 651300-52-6P
651302-21-5P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(review of application and preparation of organometallic complexes of zirconium and hafnium)

IT 83-33-0P 92-52-4P, 1,1'-Biphenyl, preparation 101-81-5P 111-83-1P
111-85-3P 122-97-4P, Benzenepropanol 124-18-5P, Decane 485-43-8P
496-11-7P 585-74-0P 586-37-8P 629-27-6P 694-35-9P 770-09-2P
886-66-8P 1273-01-4P 1528-30-9P 2243-27-8P, Nonanenitrile
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5187-81-5P 5808-05-9P 7302-03-6P 7317-52-4P 7450-04-6P
11059-81-7P 11082-39-6P 12109-84-1P 13043-55-5P 13154-13-7P
13343-78-7P 13343-79-8P 13343-80-1P 15036-22-3P 15673-05-9P
17938-20-4P 17938-58-8P 18277-20-8P, 7,9-Hexadecadiyne 18829-56-6P
19141-40-3P 20218-42-2P 20452-78-2P 20565-86-0P **20859-11-4P**
21823-66-5P 24356-02-3P 25284-37-1P 27799-31-1P 31406-67-4P
31756-35-1P 32665-18-2P 33091-15-5P 36547-88-3P 37260-83-6P
37260-85-8P 37490-22-5P 38010-72-9P 39413-64-4P 39413-75-7P
40841-79-0P 41496-82-6P 41558-36-5P 42077-14-5P 50397-92-7P
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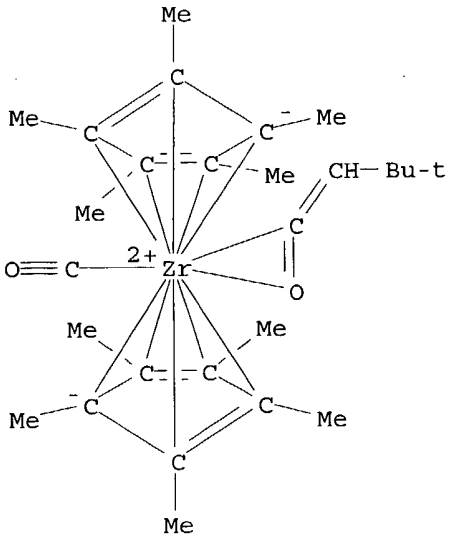
130663-93-3P 130882-82-5P 131145-64-7P 132079-31-3P 132100-80-2P
132100-81-3P 132514-23-9P 132833-06-8P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(review of application and preparation of organometallic complexes of zirconium and hafnium)

IT **84987-26-8**
RL: **CAT (Catalyst use)**; RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(review of application and preparation of organometallic complexes of zirconium and hafnium)

RN 84987-26-8 HCAPLUS
CN Zirconium, carbonyl[(0,1-η)-3,3-dimethyl-1-buten-1-one]bis[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]- (9CI) (CA INDEX NAME)



IT **7440-58-6DP**, Hafnium, organometallic complexes **7440-67-7DP**

, Zirconium, organometallic complexes
RL: **CAT (Catalyst use)**; RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(review of application and preparation of organometallic complexes of zirconium and hafnium)

RN 7440-58-6 HCAPLUS
CN Hafnium (8CI, 9CI) (CA INDEX NAME)

Hf

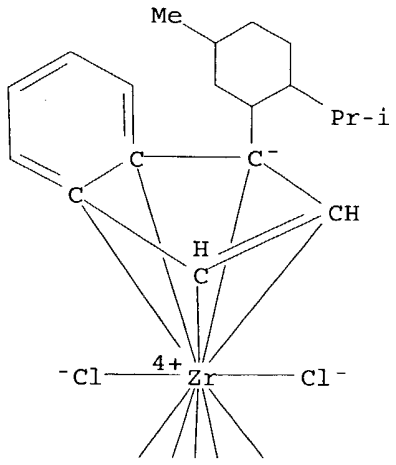
RN 7440-67-7 HCAPLUS
CN Zirconium (8CI, 9CI) (CA INDEX NAME)

Zr

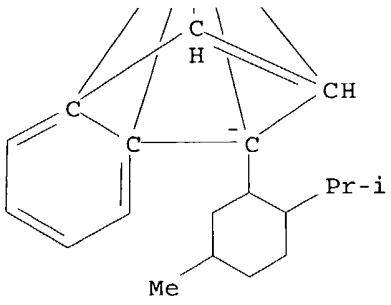
IT **148276-57-7P 148347-89-1P 148347-91-5P 148347-92-6P**
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(review of application and preparation of organometallic complexes of zirconium and hafnium)

RN 148276-57-7 HCAPLUS
CN Zirconium, dichlorobis[(1,2,3,3a,7a-η)-1-[5-methyl-2-(1-methylethyl)cyclohexyl]-1H-inden-1-yl]-, stereoisomer (9CI) (CA INDEX NAME)

PAGE 1-A

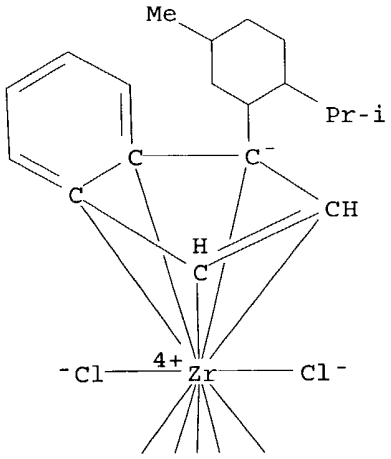


PAGE 2-A

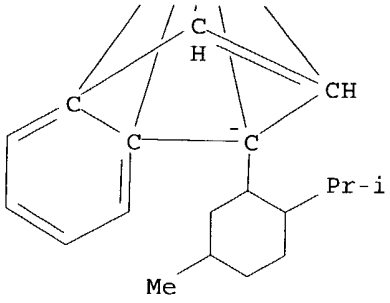


RN 148347-89-1 HCAPLUS
CN Zirconium, dichlorobis[(1,2,3,3a,7a-η)-1-[5-methyl-2-(1-methylethyl)cyclohexyl]-1H-inden-1-yl]-, stereoisomer (9CI) (CA INDEX NAME)

PAGE 1-A

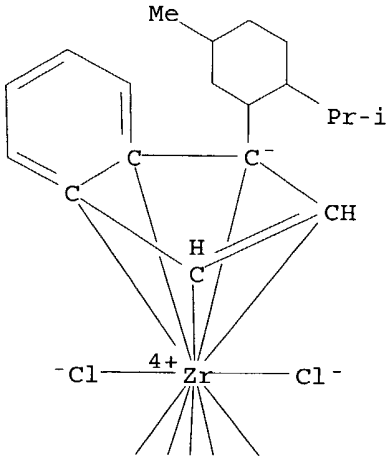


PAGE 2-A



RN 148347-91-5 HCAPLUS
CN Zirconium, dichlorobis[(1,2,3,3a,7a-η)-1-[5-methyl-2-(1-methylethyl)cyclohexyl]-1H-inden-1-yl]-, stereoisomer (9CI) (CA INDEX NAME)

PAGE 1-A



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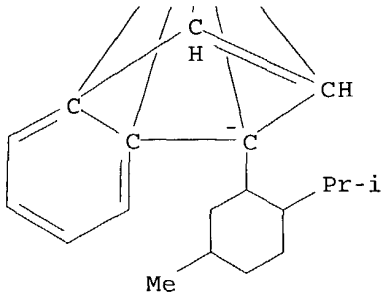
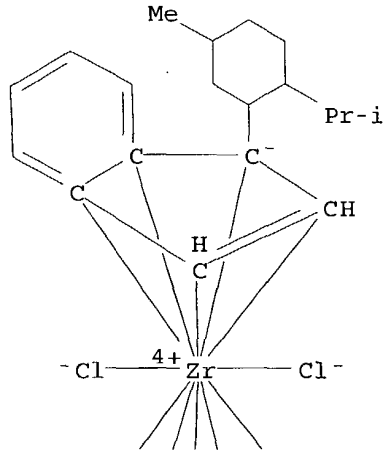
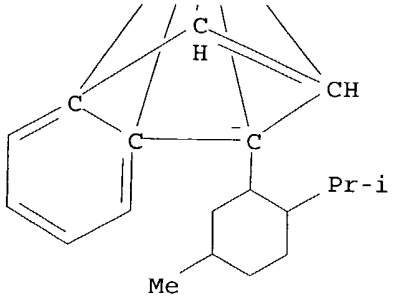


RN 148347-92-6 HCAPLUS
CN Zirconium, dichlorobis[(1,2,3,3a,7a-η)-1-[5-methyl-2-(1-methylethyl)cyclohexyl]-1H-inden-1-yl]-, stereoisomer (9CI) (CA INDEX NAME)

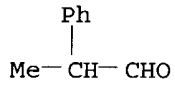
PAGE 1-A



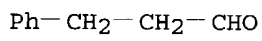


IT **93-53-8 104-53-0**, Benzenepropanal **123-38-6**, Propanal, reactions **124-13-0**, Octanal **502-56-7**, 5-Nonanone **617-35-6 6213-87-2 50396-96-8 70304-14-2 155167-77-4 155835-37-3 157835-98-8**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(review of application and preparation of organometallic complexes of zirconium and hafnium)

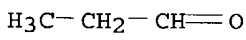
RN 93-53-8 HCAPLUS
CN Benzeneacetaldehyde, α-methyl- (9CI) (CA INDEX NAME)



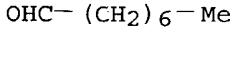
RN 104-53-0 HCAPLUS
CN Benzenepropanal (9CI) (CA INDEX NAME)



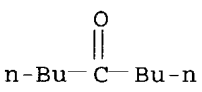
RN 123-38-6 HCAPLUS
CN Propanal (9CI) (CA INDEX NAME)



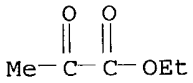
RN 124-13-0 HCAPLUS
CN Octanal (8CI, 9CI) (CA INDEX NAME)



RN 502-56-7 HCAPLUS
CN 5-Nonanone (6CI, 8CI, 9CI) (CA INDEX NAME)

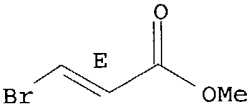


RN 617-35-6 HCAPLUS
CN Propanoic acid, 2-oxo-, ethyl ester (9CI) (CA INDEX NAME)



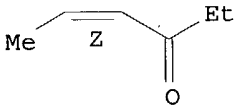
RN 6213-87-2 HCAPLUS
CN 2-Propenoic acid, 3-bromo-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

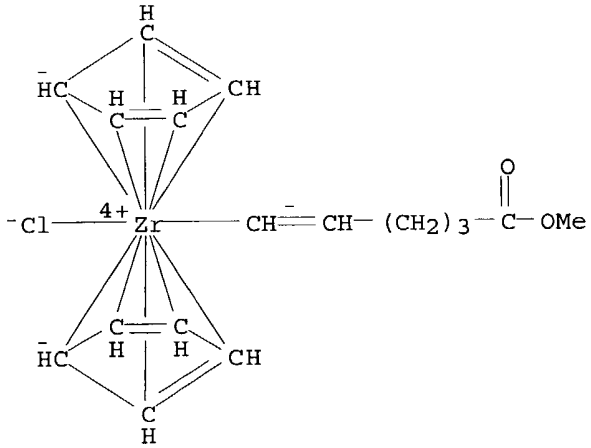


RN 50396-96-8 HCAPLUS
CN 4-Hexen-3-one, (4Z)- (9CI) (CA INDEX NAME)

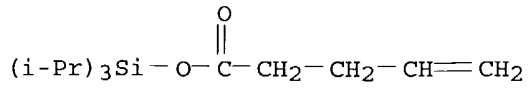
Double bond geometry as shown.



RN 70304-14-2 HCAPLUS
CN Zirconium, chlorobis(η5-2,4-cyclopentadien-1-yl)[(1E)-6-methoxy-6-oxo-1-hexenyl]- (9CI) (CA INDEX NAME)

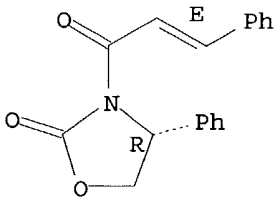


RN 155167-77-4 HCAPLUS
CN 4-Pentenoic acid, tris(1-methylethyl)silyl ester (9CI) (CA INDEX NAME)

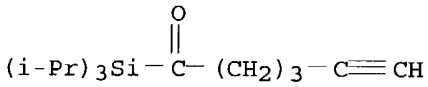


RN 155835-37-3 HCAPLUS
CN 2-Oxazolidinone, 3-[(2E)-1-oxo-3-phenyl-2-propenyl]-4-phenyl-, (4R)- (9CI) (CA INDEX NAME)

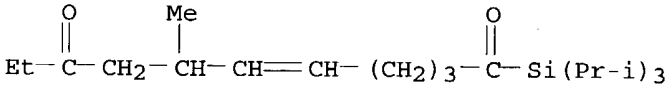
Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



RN 157835-98-8 HCAPLUS
CN Silane, tris(1-methylethyl)(1-oxo-5-hexynyl)- (9CI) (CA INDEX NAME)

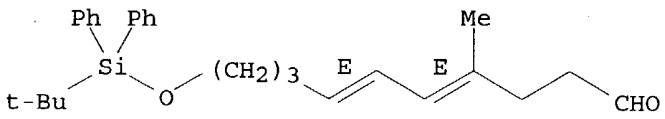


IT **157836-00-5P 180866-33-5P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(review of application and preparation of organometallic complexes of zirconium and hafnium)
RN 157836-00-5 HCAPLUS
CN 6-Undecen-3-one, 5-methyl-11-oxo-11-[tris(1-methylethyl)silyl]- (9CI) (CA INDEX NAME)



RN 180866-33-5 HCAPLUS
CN 4,6-Decadienal, 10-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-4-methyl-, (4E,6E)- (9CI) (CA INDEX NAME)

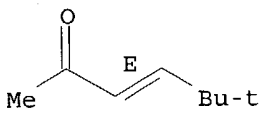
Double bond geometry as shown.



IT **20859-11-4P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**

(review of application and preparation of organometallic complexes of zirconium and hafnium)
RN 20859-11-4 HCAPLUS
CN 3-Hexen-2-one, 5,5-dimethyl-, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 488 THERE ARE 488 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:906114 HCAPLUS
DOCUMENT NUMBER: 138:4201
TITLE: Catalytic system for aldol reactions
INVENTOR(S): Jacoby, Denis
PATENT ASSIGNEE(S): Firmenich Sa, Switz.
SOURCE: PCT Int. Appl., 19 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002094755	A1	20021128	WO 2002-IB1839	20020521
W: CN, IL, IN, JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
EP 1395542	A1	20040310	EP 2002-730616	20020521
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
US 2004082818	A1	20040429	US 2003-688297	20031017

PRIORITY APPLN. INFO.: WO 2001-IB902 W 20010522
WO 2002-IB1839 W 20020521

OTHER SOURCE(S): CASREACT 138:4201; MARPAT 138:4201

AB The invention relates to a process for the preparation, in a single step, of enones by an aldol condensation of a ketone, such as a gem-dimethylcyclohexylethanone or gem-dimethylcyclohexenylethanone derivative, with an aldehyde in the presence of a novel catalytic system and without the pre-formation of an enolate. Said catalytic system consists of a metal complex, such as a [(Cl)n(alkoxy)4-nTi] or [(Cl)n(alkoxy)4-nZr] complex (n = 1-3), and a co-ingredient, such as a carboxylic acid anhydride or an anhydrous salt. Thus, 1-(2,6,6-trimethyl-3-cyclohexen-1-yl)-1-ethanone was treated with MeCHO in presence of Zr(OPr)Cl3 and MgCl2 to give 45% 1-(2,6,6-trimethyl-3-cyclohexen-1-yl)-2-buten-1-one.

IC ICM C07C045-72
ICS C07C049-557; B01J031-12

CC 21-2 (General Organic Chemistry)

IT 106-31-0, Butyric anhydride 108-24-7, Acetic anhydride 123-62-6, Propionic anhydride **3981-83-7**, Isopropoxytitanium trichloride 7637-07-2, Boron trifluoride, uses 7705-08-0, Iron(III) chloride, uses

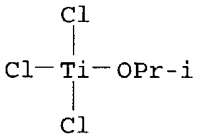
7757-82-6, Sodium sulfate, uses 7778-80-5, Potassium sulfate, uses
7786-30-3, Magnesium chloride, uses **31676-28-5**,
Dipropoxyzirconium dichloride **113133-11-2**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalytic system for aldol reactions)

IT **50-00-0**, Formaldehyde, reactions **75-07-0**, Acetaldehyde,
reactions **78-93-3**, 2-Butanone, reactions **107-02-8**,
2-Propenal, reactions 830-13-7, Cyclododecanone 1193-47-1,
2,2-Dimethylcyclohexanone **1197-92-8 4170-30-3**,
2-Butenal **37709-66-3 41435-93-2 41436-46-8**
54201-08-0 55981-43-6 73956-68-0
91819-58-8 476689-60-8 476689-61-9
476689-64-2 476689-65-3
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(catalytic system for aldol reactions)

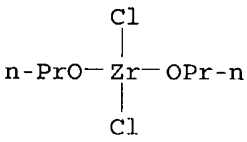
IT **565-62-8P** 23696-85-7P 57020-37-8P 65113-95-3P 83218-16-0P
255058-92-5P 344296-64-6P 476689-62-0P 476689-63-1P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(catalytic system for aldol reactions)

IT **3981-83-7**, Isopropoxytitanium trichloride **31676-28-5**,
Dipropoxyzirconium dichloride **113133-11-2**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalytic system for aldol reactions)

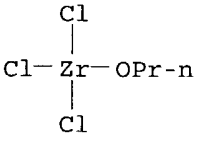
RN 3981-83-7 HCAPLUS
CN Titanium, trichloro(2-propanolato)-, (T-4)- (9CI) (CA INDEX NAME)



RN 31676-28-5 HCAPLUS
CN Zirconium, dichlorodipropoxy-, (T-4)- (9CI) (CA INDEX NAME)



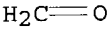
RN 113133-11-2 HCAPLUS
CN Zirconium, trichloropropoxy-, (T-4)- (9CI) (CA INDEX NAME)



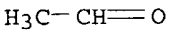
IT **50-00-0**, Formaldehyde, reactions **75-07-0**, Acetaldehyde,
reactions **78-93-3**, 2-Butanone, reactions **107-02-8**,
2-Propenal, reactions **1197-92-8 4170-30-3**, 2-Butenal

37709-66-3 41435-93-2 41436-46-8
54201-08-0 55981-43-6 73956-68-0
91819-58-8 476689-60-8 476689-61-9
476689-64-2 476689-65-3
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(catalytic system for aldol reactions)

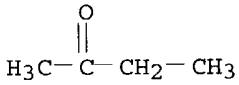
RN 50-00-0 HCAPLUS
CN Formaldehyde (8CI, 9CI) (CA INDEX NAME)



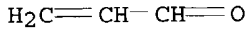
RN 75-07-0 HCAPLUS
CN Acetaldehyde (8CI, 9CI) (CA INDEX NAME)



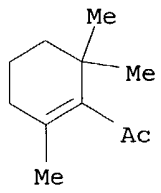
RN 78-93-3 HCAPLUS
CN 2-Butanone (8CI, 9CI) (CA INDEX NAME)



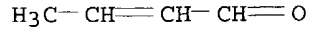
RN 107-02-8 HCAPLUS
CN 2-Propenal (9CI) (CA INDEX NAME)



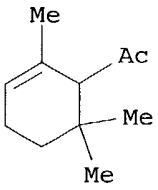
RN 1197-92-8 HCAPLUS
CN Ethanone, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



RN 4170-30-3 HCAPLUS
CN 2-Butenal (9CI) (CA INDEX NAME)

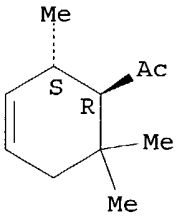


RN 37709-66-3 HCAPLUS
CN Ethanone, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)

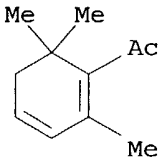


RN 41435-93-2 HCAPLUS
CN Ethanone, 1-[(1R,2S)-2,6,6-trimethyl-3-cyclohexen-1-yl]-, rel- (9CI) (CA INDEX NAME)

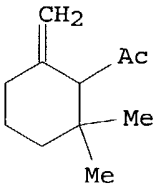
Relative stereochemistry.



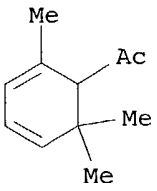
RN 41436-46-8 HCAPLUS
CN Ethanone, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)- (9CI) (CA INDEX NAME)



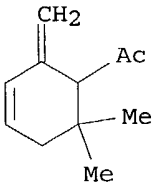
RN 54201-08-0 HCAPLUS
CN Ethanone, 1-(2,2-dimethyl-6-methylenecyclohexyl)- (9CI) (CA INDEX NAME)



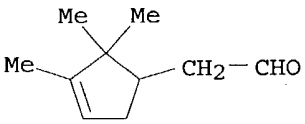
RN 55981-43-6 HCAPLUS
CN Ethanone, 1-(2,6,6-trimethyl-2,4-cyclohexadien-1-yl)- (9CI) (CA INDEX NAME)



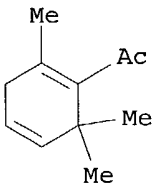
RN 73956-68-0 HCAPLUS
CN Ethanone, 1-(6,6-dimethyl-2-methylene-3-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



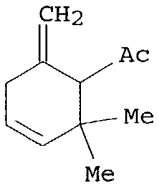
RN 91819-58-8 HCAPLUS
CN 3-Cyclopentene-1-acetaldehyde, 2,2,3-trimethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



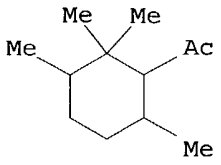
RN 476689-60-8 HCAPLUS
CN Ethanone, 1-(2,6,6-trimethyl-1,4-cyclohexadien-1-yl)- (9CI) (CA INDEX NAME)



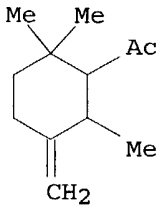
RN 476689-61-9 HCAPLUS
CN Ethanone, 1-(2,2-dimethyl-6-methylene-3-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



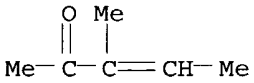
RN 476689-64-2 HCAPLUS
CN Ethanone, 1-(2,2,3,6-tetramethylcyclohexyl)- (9CI) (CA INDEX NAME)



RN 476689-65-3 HCAPLUS
CN Ethanone, 1-(2,2,6-trimethyl-5-methylenecyclohexyl)- (9CI) (CA INDEX NAME)



IT **565-62-8P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(catalytic system for aldol reactions)
RN 565-62-8 HCAPLUS
CN 3-Penten-2-one, 3-methyl- (8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:821889 HCAPLUS
DOCUMENT NUMBER: 136:118295
TITLE: Stereoselective synthesis of δ-lactones from 5-oxoalkanals via one-pot sequential acetalization, Tishchenko reaction, and lactonization by cooperative catalysis of samarium ion and mercaptan
AUTHOR(S): Hsu, Jue-Liang; Fang, Jim-Min

CORPORATE SOURCE: Department of Chemistry, National Taiwan University, Taipei, 106, Taiwan
SOURCE: Journal of Organic Chemistry (2001), 66(25), 8573-8584
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB By the synergistic catalysis of samarium ion and mercaptan, a series of 5-oxoalkanals was converted to (substituted) δ-lactones in efficient and stereoselective manners. This one-pot procedure comprises a sequence of acetalization, Tishchenko reaction and lactonization. The deliberative use of mercaptan, by comparison with alc., is advantageous to facilitate the catalytic cycle. The reaction mechanism and stereochem. are proposed and supported by some exptl. evidence. Such samarium ion/mercaptan cocatalyzed reactions show the feature of remote control, which is applicable to the asym. synthesis of optically active δ-lactones. This study also demonstrates the synthesis of two insect pheromones, (2S,5R)-2-methylhexanolide and (R)-hexadecanolide, as examples of a new protocol for asym. reduction of long-chain aliphatic ketones.

CC 26-2 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 67, 75

IT 555-31-7, Aluminum triisopropoxide 624-92-0 882-33-7 2263-49-2 3504-40-3, Samarium triisopropoxide 4253-89-8 7440-19-9D, Samarium, ion, uses 10361-82-7, Samarium trichloride 10465-27-7, Samarium triacetate 13759-87-0, Samarium tribromide 13765-24-7, Samarium trifluoride **22378-84-3**, Titanium triisopropoxide 32248-43-4, Samarium diiodide
RL: **CAT (Catalyst use)**; USES (Uses)
(one-pot sequential acetalization, Tishchenko reaction, and lactonization by the promotion of samarium ion and mercaptans in stereoselective synthesis of δ-lactones from 5-oxoalkanals)

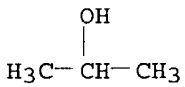
IT 57-14-7 57-88-5, Cholesterol, reactions 67-63-0, Isopropanol, reactions 75-33-2, Isopropyl thiol 75-77-4, Trimethylsilyl chloride, reactions **75-97-8 78-84-2** 98-91-9, Thiobenzoic acid 100-39-0, Benzyl bromide **100-52-7**, Benzaldehyde, reactions 100-58-3, Phenyl magnesium bromide 104-92-7, 4-Methoxyphenyl bromide **107-02-8**, Acrolein, reactions 108-86-1, Bromobenzene, reactions 111-24-0, 1,5-Dibromopentane 111-25-1, n-Hexyl bromide 111-83-1, n-Octyl bromide 120-92-3, Cyclopentanone **123-38-6**, Propanal, reactions 299-42-3, (-)-Ephedrine 492-41-1, (-)-Norephedrine 603-35-0, Triphenylphosphine, reactions 676-58-4, Methylmagnesium chloride 925-90-6, Ethylmagnesiumbromide 931-50-0, Cyclohexyl magnesium bromide 2216-51-5, (-)-Menthol 2216-52-6, (+)-Neomenthol 3144-16-9 **4170-30-3**, Crotonaldehyde 5162-44-7 6672-30-6 7440-19-9, Samarium, reactions 7553-56-2, Iodine, reactions 23364-44-5 24041-60-9, (+)-Isopinocampheol 53750-52-0 58911-63-0 59983-39-0, (S)-1-Amino-2-(methoxymethyl)pyrrolidine 65253-04-5, (-)-8-Phenylmenthol 72203-94-2 **75424-65-6** 83665-55-8, 2-(2-Iodoethyl)-1,3-dioxolane **88072-97-3** 88303-25-7, Tetradecyl magnesium bromide 92206-73-0, Octadecyl magnesium bromide 117286-10-9, Undecylmagnesium bromide 162204-10-6 **389837-65-4** 389837-86-9
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(one-pot sequential acetalization, Tishchenko reaction, and lactonization by the promotion of samarium ion and mercaptans in stereoselective synthesis of δ-lactones from 5-oxoalkanals)

IT **78-94-4P**, 3-Buten-2-one, preparation **505-03-3P** 825-54-7P **1443-86-3P 2226-27-9P** 2230-82-2P **2552-91-2P 2568-20-9P** 13148-28-2P **13544-11-1P** 61091-40-5P 61347-76-0P 69498-77-7P **74327-34-7P**

75424-63-4P 95664-94-1P 111183-87-0P
111183-88-1P 120017-08-5P 124851-49-6P
133522-23-3P **253869-05-5P 253869-14-6P**
389837-23-4P 389837-58-5P 389837-59-6P
389837-60-9P 389837-61-0P 389837-64-3P
389837-67-6P 389837-68-7P 389837-69-8P
389837-70-1P 389837-77-8P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; **RACT (Reactant or reagent)**
(one-pot sequential acetalization, Tishchenko reaction, and lactonization by the promotion of samarium ion and mercaptans in stereoselective synthesis of δ-lactones from 5-oxoalkanals)

IT **22378-84-3**, Titanium triisopropoxide
RL: **CAT (Catalyst use)**; USES (Uses)
(one-pot sequential acetalization, Tishchenko reaction, and lactonization by the promotion of samarium ion and mercaptans in stereoselective synthesis of δ-lactones from 5-oxoalkanals)

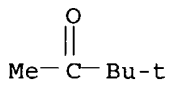
RN 22378-84-3 HCAPLUS
CN 2-Propanol, titanium(3+) salt (9CI) (CA INDEX NAME)



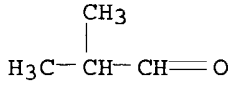
●1/3 Ti(III)

IT **75-97-8 78-84-2 100-52-7**, Benzaldehyde, reactions **107-02-8**, Acrolein, reactions **123-38-6**, Propanal, reactions **4170-30-3**, Crotonaldehyde **75424-65-6 88072-97-3 389837-65-4**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(one-pot sequential acetalization, Tishchenko reaction, and lactonization by the promotion of samarium ion and mercaptans in stereoselective synthesis of δ-lactones from 5-oxoalkanals)

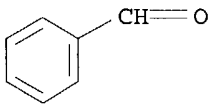
RN 75-97-8 HCAPLUS
CN 2-Butanone, 3,3-dimethyl- (8CI, 9CI) (CA INDEX NAME)



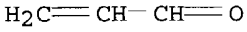
RN 78-84-2 HCAPLUS
CN Propanal, 2-methyl- (9CI) (CA INDEX NAME)



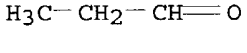
RN 100-52-7 HCAPLUS
CN Benzaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



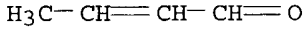
RN 107-02-8 HCAPLUS
CN 2-Propenal (9CI) (CA INDEX NAME)



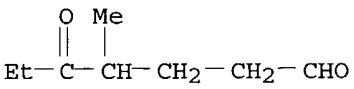
RN 123-38-6 HCAPLUS
CN Propanal (9CI) (CA INDEX NAME)



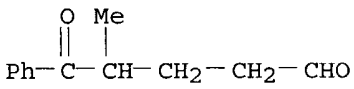
RN 4170-30-3 HCAPLUS
CN 2-Butenal (9CI) (CA INDEX NAME)



RN 75424-65-6 HCAPLUS
CN Heptanal, 4-methyl-5-oxo- (9CI) (CA INDEX NAME)

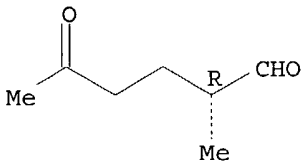


RN 88072-97-3 HCAPLUS
CN Benzenepentanal, γ-methyl-δ-oxo- (9CI) (CA INDEX NAME)



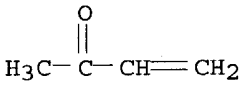
RN 389837-65-4 HCAPLUS
CN Hexanal, 2-methyl-5-oxo-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

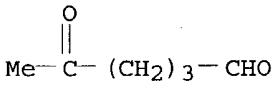


IT **78-94-4P**, 3-Buten-2-one, preparation **505-03-3P**
1443-86-3P 2226-27-9P 2552-91-2P
2568-20-9P 13544-11-1P 74327-34-7P
75424-63-4P 95664-94-1P 111183-87-0P
111183-88-1P 120017-08-5P 124851-49-6P
253869-05-5P 253869-14-6P 389837-23-4P
389837-58-5P 389837-59-6P 389837-60-9P
389837-61-0P 389837-64-3P 389837-67-6P
389837-68-7P 389837-69-8P 389837-70-1P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; **RACT (Reactant or reagent)**
(one-pot sequential acetalization, Tishchenko reaction, and lactonization by the promotion of samarium ion and mercaptans in stereoselective synthesis of δ-lactones from 5-oxoalkanals)

RN 78-94-4 HCAPLUS
CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)

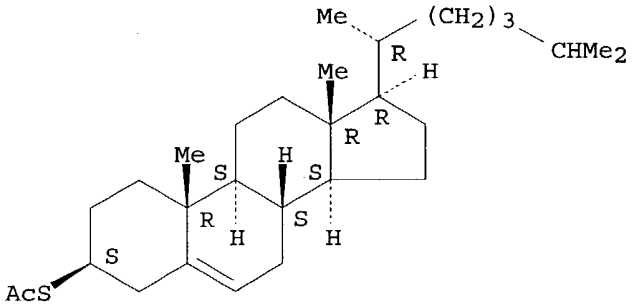


RN 505-03-3 HCAPLUS
CN Hexanal, 5-oxo- (7CI, 8CI, 9CI) (CA INDEX NAME)



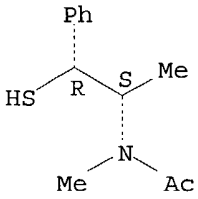
RN 1443-86-3 HCAPLUS
CN Cholest-5-ene-3-thiol, acetate, (3β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



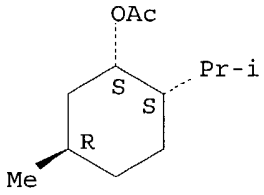
RN 2226-27-9 HCAPLUS
CN Acetamide, N-[(1S,2R)-2-mercapto-1-methyl-2-phenylethyl]-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

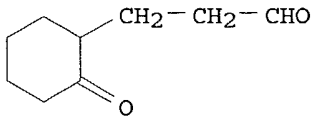


RN 2552-91-2 HCAPLUS
CN Cyclohexanol, 5-methyl-2-(1-methylethyl)-, acetate, (1S,2S,5R)- (9CI) (CA INDEX NAME)

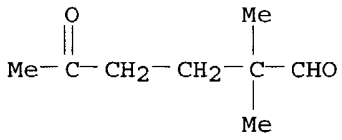
Absolute stereochemistry. Rotation (+).



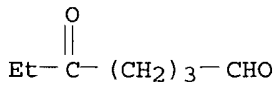
RN 2568-20-9 HCAPLUS
CN Cyclohexanepropanal, 2-oxo- (9CI) (CA INDEX NAME)



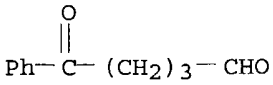
RN 13544-11-1 HCAPLUS
CN Hexanal, 2,2-dimethyl-5-oxo- (8CI, 9CI) (CA INDEX NAME)



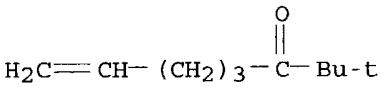
RN 74327-34-7 HCAPLUS
CN Heptanal, 5-oxo- (9CI) (CA INDEX NAME)



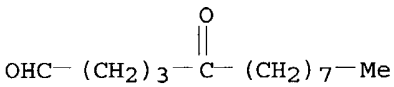
RN 75424-63-4 HCAPLUS
CN Benzenepentanal, δ-oxo- (9CI) (CA INDEX NAME)



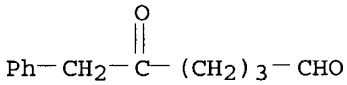
RN 95664-94-1 HCAPLUS
CN 7-Octen-3-one, 2,2-dimethyl- (9CI) (CA INDEX NAME)



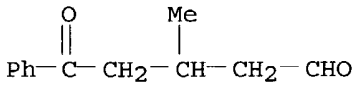
RN 111183-87-0 HCAPLUS
CN Tridecanal, 5-oxo- (9CI) (CA INDEX NAME)



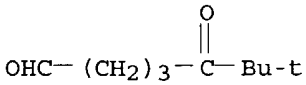
RN 111183-88-1 HCAPLUS
CN Benzenehexanal, δ-oxo- (9CI) (CA INDEX NAME)



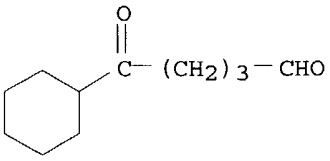
RN 120017-08-5 HCAPLUS
CN Benzenepentanal, β-methyl-δ-oxo- (9CI) (CA INDEX NAME)



RN 124851-49-6 HCAPLUS
CN Heptanal, 6,6-dimethyl-5-oxo- (9CI) (CA INDEX NAME)

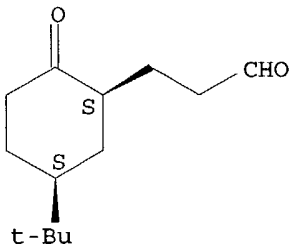


RN 253869-05-5 HCAPLUS
CN Cyclohexanepentanal, δ-oxo- (9CI) (CA INDEX NAME)



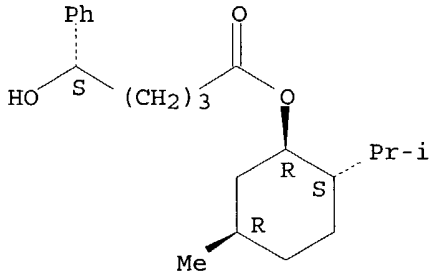
RN 253869-14-6 HCAPLUS
CN Cyclohexanepropanal, 5-(1,1-dimethylethyl)-2-oxo-, (1R,5R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

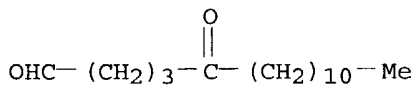


RN 389837-23-4 HCAPLUS
CN Benzenepentanoic acid, δ-hydroxy-, (1R,2S,5R)-5-methyl-2-(1-methylethyl)cyclohexyl ester, (δS)- (9CI) (CA INDEX NAME)

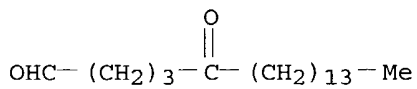
Absolute stereochemistry.



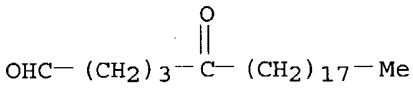
RN 389837-58-5 HCAPLUS
CN Hexadecanal, 5-oxo- (9CI) (CA INDEX NAME)



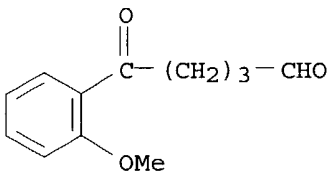
RN 389837-59-6 HCAPLUS
CN Nonadecanal, 5-oxo- (9CI) (CA INDEX NAME)



RN 389837-60-9 HCAPLUS
CN Tricosanal, 5-oxo- (9CI) (CA INDEX NAME)

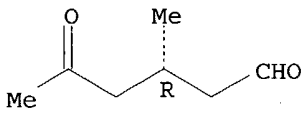


RN 389837-61-0 HCAPLUS
CN Benzenepentanal, 2-methoxy-δ-oxo- (9CI) (CA INDEX NAME)



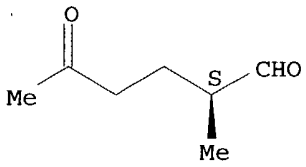
RN 389837-64-3 HCAPLUS
CN Hexanal, 3-methyl-5-oxo-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



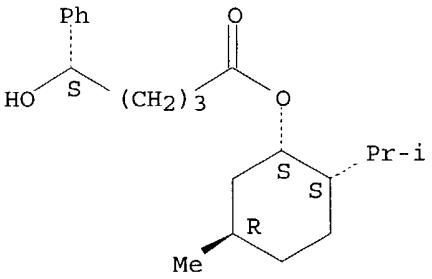
RN 389837-67-6 HCAPLUS
CN Hexanal, 2-methyl-5-oxo-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



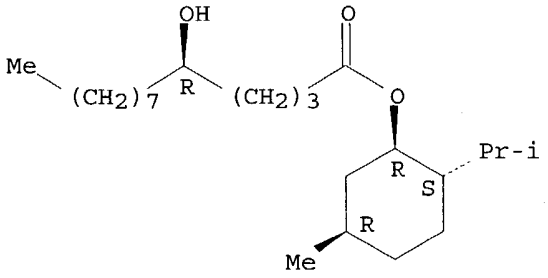
RN 389837-68-7 HCAPLUS
CN Benzenepentanoic acid, δ-hydroxy-, (1S,2S,5R)-5-methyl-2-(1-methylethyl)cyclohexyl ester, (δS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



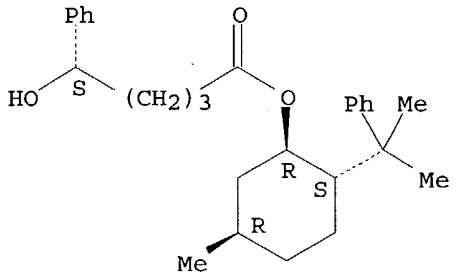
RN 389837-69-8 HCAPLUS
CN Tridecanoic acid, 5-hydroxy-, (1R,2S,5R)-5-methyl-2-(1-methylethyl)cyclohexyl ester, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 389837-70-1 HCAPLUS
CN Benzenepentanoic acid, δ-hydroxy-, (1R,2S,5R)-5-methyl-2-(1-methyl-1-phenylethyl)cyclohexyl ester, (δS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 104 THERE ARE 104 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:845875 HCAPLUS
DOCUMENT NUMBER: 134:147145
TITLE: A straightforward synthesis of cyclopropanes from aldehydes and ketones
AUTHOR(S): Gandon, Vincent; Bertus, Philippe; Szymoniak, Jan
CORPORATE SOURCE: CNRS UMR 6519 "Reactions selectives et applications",

Universite de Reims-Champagne-Ardenne, Reims, 51687, Fr.
SOURCE: European Journal of Organic Chemistry (2000), (22), 3713-3719
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:147145

AB A new synthetic methodol. for preparing cyclopropanes is presented. The reaction involves a cooperative zirconium- and Lewis acid-mediated deoxygenative coupling of carbonyl compds. with a Grignard reagent. In this way, various cyclopropanes are obtained in moderate to excellent yields, directly from saturated, unsatd., and aromatic aldehydes and ketones. This reaction tolerates the presence of several different functional groups. For example, the deoxidn./coupling of 1-(2-naphthalenyl)ethanone with ethylmagnesium bromide gave 2-(1-methylcyclopropyl)naphthalene; the similar reaction of 2-naphthalenecarboxaldehyde gave 2-cyclopropylnaphthalene. In contrast, the reaction of 1-(2-naphthalenyl)ethanone or 2-(1-methylcyclopropyl)naphthalene with zirconocene dichloride/sulfuric acid gave α-ethyl-α-methyl-2-naphthalenemethanol or α-ethyl-2-naphthalenemethanol, resp. The chemoselective reaction of N-methyl-γ-oxo-N-(phenylmethyl)benzenebutanamide with ethylmagnesium bromide gave N-Methyl-1-phenyl-N-(phenylmethyl)cyclopropanepropanamide.

CC 21-2 (General Organic Chemistry)

IT **1291-32-3**, Zirconocene dichloride **7550-45-0**, Titanium chloride (TiCL4), uses
RL: **CAT (Catalyst use)**; USES (Uses)
(preparation of cyclopropane derivs. by deoxygenation and coupling of aldehydes or ketones and Grignard reagent)

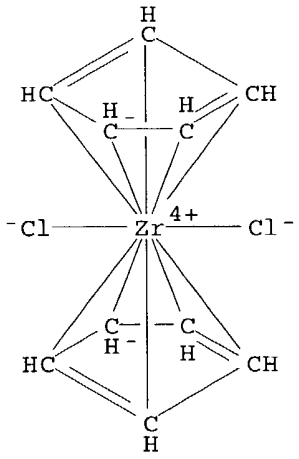
IT **57-83-0**, Pregn-4-ene-3,20-dione, reactions **66-99-9**, 2-Naphthalenecarboxaldehyde 78-59-1, 3,5,5-Trimethyl-2-cyclohexen-1-one **93-08-3**, 1-(2-Naphthalenyl)ethanone 103-67-3, N-Methylbenzylamine **112-12-9**, 2-Undecanone **112-61-8**, Methyl stearate **123-11-5**, 4-Methoxybenzaldehyde, reactions 601-57-0, Cholest-4-en-3-one **638-66-4**, Octadecanal **768-03-6**, 1-Phenyl-2-propen-1-one 925-90-6, Ethylmagnesium bromide 927-77-5, Propylmagnesium bromide **1896-62-4**, (E)-4-Phenyl-3-buten-2-one **2051-95-8**, β-Benzoylpropionic acid **3913-81-3**, (E)-2-Decenal **5392-40-5** 7152-03-6, Methanone cyclopropyl(4-methoxyphenyl) **14371-10-9** 15600-08-5, Cholestan-3-one 20007-72-1 **33603-90-6** 51051-65-1 54458-61-6, 2,3,4,5-Tetramethyl-2-cyclopenten-1-one **58879-39-3**, 1-Dodecen-3-one
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(preparation of cyclopropane derivs. by deoxygenation and coupling of aldehydes or ketones and Grignard reagent)

IT 978-98-3P **101729-68-4P 252188-57-1P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; **RACT (Reactant or reagent)**
(preparation of cyclopropane derivs. by deoxygenation and coupling of aldehydes or ketones and Grignard reagent)

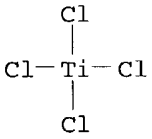
IT **1291-32-3**, Zirconocene dichloride **7550-45-0**, Titanium chloride (TiCL4), uses
RL: **CAT (Catalyst use)**; USES (Uses)
(preparation of cyclopropane derivs. by deoxygenation and coupling of aldehydes or ketones and Grignard reagent)

RN 1291-32-3 HCAPLUS

CN Zirconium, dichlorobis(η5-2,4-cyclopentadien-1-yl)- (9CI) (CA INDEX NAME)

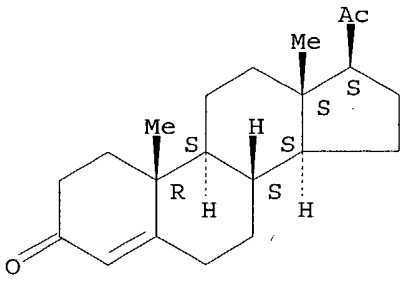


RN 7550-45-0 HCAPLUS
CN Titanium chloride (TiCl4) (T-4)- (9CI) (CA INDEX NAME)

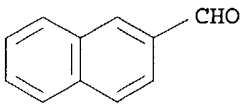


IT **57-83-0**, Pregn-4-ene-3,20-dione, reactions **66-99-9**, 2-Naphthalenecarboxaldehyde **93-08-3**, 1-(2-Naphthalenyl)ethanone **112-12-9**, 2-Undecanone **112-61-8**, Methyl stearate **123-11-5**, 4-Methoxybenzaldehyde, reactions **638-66-4**, Octadecanal **768-03-6**, 1-Phenyl-2-propen-1-one **1896-62-4**, (E)-4-Phenyl-3-buten-2-one **2051-95-8**, β-Benzoylpropionic acid **3913-81-3**, (E)-2-Decenal **5392-40-5** **14371-10-9** **33603-90-6** **58879-39-3**, 1-Dodecen-3-one
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(preparation of cyclopropane derivs. by deoxygenation and coupling of aldehydes or ketones and Grignard reagent)
RN 57-83-0 HCAPLUS
CN Pregn-4-ene-3,20-dione (9CI) (CA INDEX NAME)

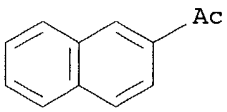
Absolute stereochemistry.



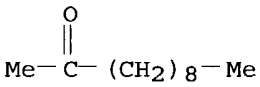
RN 66-99-9 HCAPLUS
CN 2-Naphthalenecarboxaldehyde (9CI) (CA INDEX NAME)



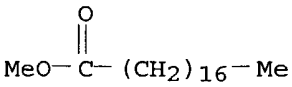
RN 93-08-3 HCAPLUS
CN Ethanone, 1-(2-naphthalenyl)- (9CI) (CA INDEX NAME)



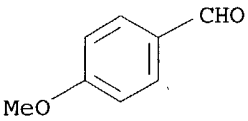
RN 112-12-9 HCAPLUS
CN 2-Undecanone (6CI, 8CI, 9CI) (CA INDEX NAME)



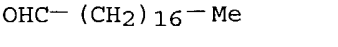
RN 112-61-8 HCAPLUS
CN Octadecanoic acid, methyl ester (9CI) (CA INDEX NAME)



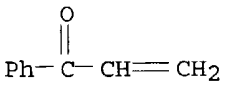
RN 123-11-5 HCAPLUS
CN Benzaldehyde, 4-methoxy- (9CI) (CA INDEX NAME)



RN 638-66-4 HCAPLUS
CN Octadecanal (9CI) (CA INDEX NAME)

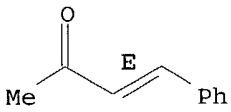


RN 768-03-6 HCAPLUS
CN 2-Propen-1-one, 1-phenyl- (9CI) (CA INDEX NAME)

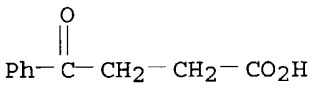


RN 1896-62-4 HCAPLUS
CN 3-Buten-2-one, 4-phenyl-, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

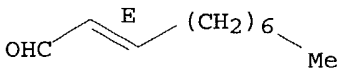


RN 2051-95-8 HCAPLUS
CN Benzenebutanoic acid, γ-oxo- (9CI) (CA INDEX NAME)

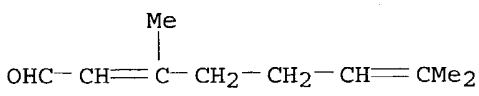


RN 3913-81-3 HCAPLUS
CN 2-Decenal, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

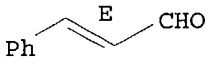


RN 5392-40-5 HCAPLUS
CN 2,6-Octadienal, 3,7-dimethyl- (8CI, 9CI) (CA INDEX NAME)



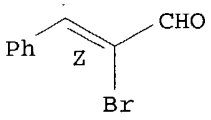
RN 14371-10-9 HCAPLUS
CN 2-Propenal, 3-phenyl-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

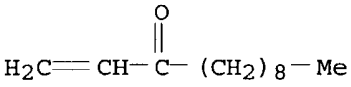


RN 33603-90-6 HCAPLUS
CN 2-Propenal, 2-bromo-3-phenyl-, (2Z)- (9CI) (CA INDEX NAME)

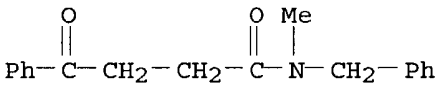
Double bond geometry as shown.



RN 58879-39-3 HCAPLUS
CN 1-Dodecen-3-one (9CI) (CA INDEX NAME)

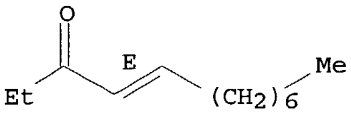


IT **101729-68-4P 252188-57-1P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; **RACT (Reactant or reagent)**
(preparation of cyclopropane derivs. by deoxygenation and coupling of aldehydes or ketones and Grignard reagent)
RN 101729-68-4 HCAPLUS
CN Benzenebutanamide, N-methyl-γ-oxo-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 252188-57-1 HCAPLUS
CN 4-Dodecen-3-one, (4E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



~~REFERENCE COUNT:~~ 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 7 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1993:408363 HCAPLUS
DOCUMENT NUMBER: 119:8363
TITLE: Preparation of unsaturated ketones from formaldehyde and ketones

INVENTOR(S): Shimazaki, Yoshiharu; Kanbe, Hideyuki; Uejima, Rikuo
PATENT ASSIGNEE(S): Nippon Catalytic Chem Ind, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05009146	A2	19930119	JP 1991-160244	19910701

PRIORITY APPLN. INFO.: JP 1991-160244 19910701
OTHER SOURCE(S): CASREACT 119:8363; MARPAT 119:8363

AB R1(CH2)nCOCR2:CH2, CH2:CR1COCH2R2, and/or CH2:CR1COCR2:CH2 [R1, R2 = H, C1-4 alkyl, (C1-4 alkyl- and/or halo-substituted) Ph; n = 0, 1], useful as intermediates for perfumes, flavors, and polymers, are prepared by condensation of R1(CH2)nCOCH2R2 (R1, R2 = same as above) in the presence of solid catalysts of PXaOb (X = alkali metal, alkaline earth metal, Y, La, Ce, Pr, Nd, Zr, Nb, B, Si; a = 0.5-30; b = determined by the value of a) at gas phase. Gaseous acetone and HCHO were treated with PMg1.5Si5 at 350° for 1 h to give 67.5% and 7.0% (based on HCHO) Me vinyl ketone and divinyl ketone resp., vs. 28.8% and 5.4% resp., when ZrO2/SiO2 was used instead of the catalyst.

IC ICM C07C049-203
ICS B01J027-18; B01J027-182; B01J027-186; C07C045-75; C07C049-213; C07C049-227
ICA C07B061-00
CC 23-15 (Aliphatic Compounds)
Section cross-reference(s): 17, 21, 35, 62
IT 7778-53-2 13308-51-5, Boron phosphate (B(PO4)) 13573-12-1 88848-66-2 148127-13-3, Magnesium phosphorus oxide silicate (Mg1.5PO1.5(Si2O5)2.5) 148127-14-4, Calcium phosphorus oxide silicate (Ca1.5PO1.5(Si2O5)2.5) **148127-15-5**, Calcium zirconium oxide phosphate (Ca2Zr28O56.5(PO4)) 148127-16-6, Niobium strontium oxide phosphate (Nb10SrO24.5(PO4)) 148127-17-7, Barium phosphorus oxide silicate (Ba1.5PO1.5(Si2O5)2.5) **148127-18-8**, Barium zirconium oxide phosphate (Ba2Zr15O30.5(PO4)) 148127-19-9, Lithium phosphorus oxide silicate (LiPO0.5(Si2O5)2.5) 148127-20-2, Phosphorus sodium oxide silicate (PNaO0.5(Si2O5)2.5) 148127-21-3, Phosphorus potassium oxide silicate (PKO0.5(Si2O5)2.5) 148127-22-4, Phosphorus rubidium oxide silicate (PRbO0.5(Si2O5)2.5) 148127-23-5, Cesium phosphorus oxide silicate (Cs3PO1.5(Si2O5)2.5) **148127-24-6**, Cesium zirconium borate oxide phosphate (Cs2Zr5(BO3)O8(PO4)) 148127-25-7, Cesium lanthanum oxide phosphate (CsLa10O14(PO4)) **148127-26-8** 148127-27-9, Phosphorus yttrium oxide silicate (PYO1.5(Si2O5)2.5) 148127-28-0, Niobium praseodymium oxide phosphate (Nb10Pr2O26.5(PO4)) **148127-29-1**, Neodymium zirconium oxide phosphate (Nd3Zr20O43(PO4))
RL: **CAT (Catalyst use)**; USES (Uses)
(catalyst, in condensation of ketones, with formaldehyde)
IT **67-64-1**, Acetone, reactions **78-93-3**, MEK, reactions **93-55-0**, Propiophenone **96-22-0**, 3-Pentanone **98-86-2**, Acetophenone, reactions **99-91-2**, p-Chloroacetophenone **107-87-9**, Methyl propyl ketone **122-00-9**, p-Methylacetophenone
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(condensation of, with formaldehyde)
IT **50-00-0**, Formaldehyde, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**

(condensation of, with ketones)

IT **78-94-4P**, 3-Buten-2-one, preparation 768-03-6P, Vinyl phenyl ketone 769-60-8P, Phenyl isopropenyl ketone **814-78-8P**, Methyl isopropenyl ketone **1629-58-9P**, Ethyl vinyl ketone 1629-60-3P, Vinyl propyl ketone 1890-28-4P, Divinyl ketone 4359-77-7P 7448-87-5P, Vinyl p-chlorophenyl ketone 19832-78-1P, Vinyl p-methylphenyl ketone **25044-01-3P**, Ethyl isopropenyl ketone 27132-81-6P, Diisopropenyl ketone
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of, from ketone and formaldehyde)

IT **148127-15-5**, Calcium zirconium oxide phosphate (Ca2Zr28O56.5(PO4)) **148127-18-8**, Barium zirconium oxide phosphate (Ba2Zr15O30.5(PO4)) **148127-24-6**, Cesium zirconium borate oxide phosphate (Cs2Zr5(BO3)O8(PO4)) **148127-26-8 148127-29-1**, Neodymium zirconium oxide phosphate (Nd3Zr20O43(PO4))
RL: **CAT (Catalyst use)**; USES (Uses)
(catalyst, in condensation of ketones, with formaldehyde)

RN 148127-15-5 HCAPLUS
CN Calcium zirconium oxide phosphate (Ca2Zr28O56.5(PO4)) (9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
O	56.5	17778-80-2
O4P	1	14265-44-2
Ca	2	7440-70-2
Zr	28	7440-67-7

RN 148127-18-8 HCAPLUS
CN Barium zirconium oxide phosphate (Ba2Zr15O30.5(PO4)) (9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
O	30.5	17778-80-2
O4P	1	14265-44-2
Zr	15	7440-67-7
Ba	2	7440-39-3

RN 148127-24-6 HCAPLUS
CN Cesium zirconium borate oxide phosphate (Cs2Zr5(BO3)O8(PO4)) (9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
O	8	17778-80-2
O4P	1	14265-44-2
BO3	1	14213-97-9
Zr	5	7440-67-7
Cs	2	7440-46-2

RN 148127-26-8 HCAPLUS
CN Cerium lanthanum zirconium oxide phosphate (CeLaZr20O41.5(PO4)) (9CI) (CA INDEX NAME)

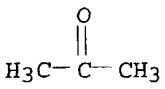
Component	Ratio	Component

		Registry Number
O	41.5	17778-80-2
O4P	1	14265-44-2
Zr	20	7440-67-7
Ce	1	7440-45-1
La	1	7439-91-0

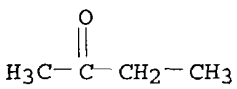
RN 148127-29-1 HCAPLUS
CN Neodymium zirconium oxide phosphate (Nd3Zr20O43(PO4)) (9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
O	43	17778-80-2
O4P	1	14265-44-2
Zr	20	7440-67-7
Nd	3	7440-00-8

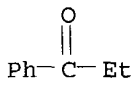
IT **67-64-1**, Acetone, reactions **78-93-3**, MEK, reactions **93-55-0**, Propiophenone **96-22-0**, 3-Pentanone **98-86-2**, Acetophenone, reactions **99-91-2**, p-Chloroacetophenone **107-87-9**, Methyl propyl ketone **122-00-9**, p-Methylacetophenone
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(condensation of, with formaldehyde)
RN 67-64-1 HCAPLUS
CN 2-Propanone (9CI) (CA INDEX NAME)



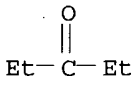
RN 78-93-3 HCAPLUS
CN 2-Butanone (8CI, 9CI) (CA INDEX NAME)



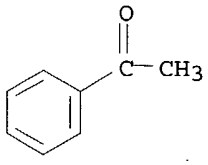
RN 93-55-0 HCAPLUS
CN 1-Propanone, 1-phenyl- (9CI) (CA INDEX NAME)



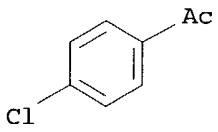
RN 96-22-0 HCAPLUS
CN 3-Pentanone (8CI, 9CI) (CA INDEX NAME)



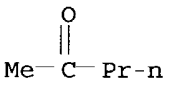
RN 98-86-2 HCAPLUS
CN Ethanone, 1-phenyl- (9CI) (CA INDEX NAME)



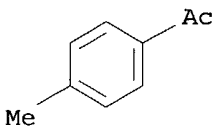
RN 99-91-2 HCAPLUS
CN Ethanone, 1-(4-chlorophenyl)- (9CI) (CA INDEX NAME)



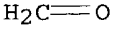
RN 107-87-9 HCAPLUS
CN 2-Pentanone (8CI, 9CI) (CA INDEX NAME)



RN 122-00-9 HCAPLUS
CN Ethanone, 1-(4-methylphenyl)- (9CI) (CA INDEX NAME)

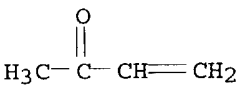


IT **50-00-0**, Formaldehyde, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(condensation of, with ketones)
RN 50-00-0 HCAPLUS
CN Formaldehyde (8CI, 9CI) (CA INDEX NAME)

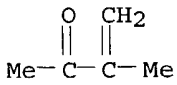


IT **78-94-4P**, 3-Buten-2-one, preparation **814-78-8P**, Methyl

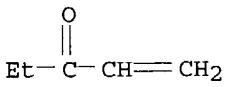
isopropenyl ketone **1629-58-9P**, Ethyl vinyl ketone **25044-01-3P**, Ethyl isopropenyl ketone
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of, from ketone and formaldehyde)
RN 78-94-4 HCAPLUS
CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



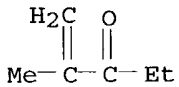
RN 814-78-8 HCAPLUS
CN 3-Buten-2-one, 3-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 1629-58-9 HCAPLUS
CN 1-Penten-3-one (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 25044-01-3 HCAPLUS
CN 1-Penten-3-one, 2-methyl- (8CI, 9CI) (CA INDEX NAME)



L32 ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1987:597115 HCAPLUS
DOCUMENT NUMBER: 107:197115
TITLE: Selective oxidation of alcohol function in allylic alcohols to α,β-unsaturated carbonyl compounds catalyzed by zirconocene complexes
AUTHOR(S): Nakano, Tatsuya; Ishii, Yasutaka; Ogawa, Masaya
CORPORATE SOURCE: Fac. Eng., Kansai Univ., Suita, 564, Japan
SOURCE: Journal of Organic Chemistry (1987), 52(22), 4855-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 107:197115
AB Cp2ZrH2 and Cp2Zr(OCHMe2)2 (Cp = cyclopentadienyl) catalyze the Oppenauer-type oxidation of allylic alcs. to α,β-unsatd. carbonyl compds in the presence of an appropriate H acceptor such as PhCHO or cyclohexanone. E.g., the primary allylic terpenoid alcs. geraniol and nerol were oxidized to 83-95% α- and β-citral, essential for

the perfumery industry. Similarly, secondary allylic alcs. such as 3-hexen-2-ol and 2-cyclohexen-1-ol were oxidized to 93% 3-hexen-2-one and 89% 2-cyclohexenone, resp. However, zirconocene complexes do not oxidize propargylic alcs.

CC 21-2 (General Organic Chemistry)
Section cross-reference(s): 62

IT **123-72-8**, Butanal **124-13-0**, Octanal
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(aldol condensation and hydride reduction of)

IT **98-01-1**, Furfural, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(aldol condensation with acetone and hydride reduction of)

IT **67-64-1**, Acetone, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(aldol condensation with furfural and hydride reduction of)

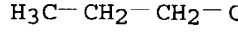
IT **37342-98-6 78091-18-6**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalyst, for oxidation of allylic alcs.)

IT 78-59-1P 106-26-3P, β-Citral 107-86-8P 123-73-9P, trans-2-Butenal 141-27-5P, α-Citral 141-79-7P 826-56-2P 930-68-7P 1629-60-3P 1896-62-4P **3102-33-8P** 4312-99-6P 6278-91-7P, 4-(Benzyloxy)-2-butanone 6728-26-3P 14371-10-9P 18977-40-7P 41438-24-8P 64344-45-2P 64935-39-3P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)

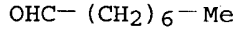
IT **78-94-4P**, preparation 107-02-8P, preparation
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of, by oxidation of allylic alc., zirconocene complex-catalyzed)

IT **123-72-8**, Butanal **124-13-0**, Octanal
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(aldol condensation and hydride reduction of)

RN 123-72-8 HCAPLUS
CN Butanal (9CI) (CA INDEX NAME)

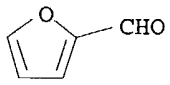


RN 124-13-0 HCAPLUS
CN Octanal (8CI, 9CI) (CA INDEX NAME)



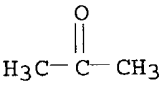
IT **98-01-1**, Furfural, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(aldol condensation with acetone and hydride reduction of)

RN 98-01-1 HCAPLUS
CN 2-Furancarboxaldehyde (9CI) (CA INDEX NAME)

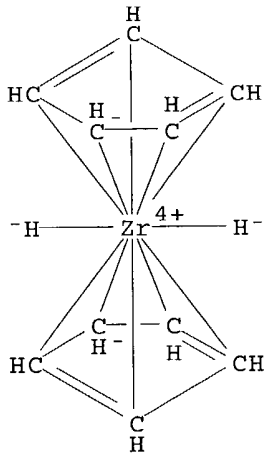


IT **67-64-1**, Acetone, reactions

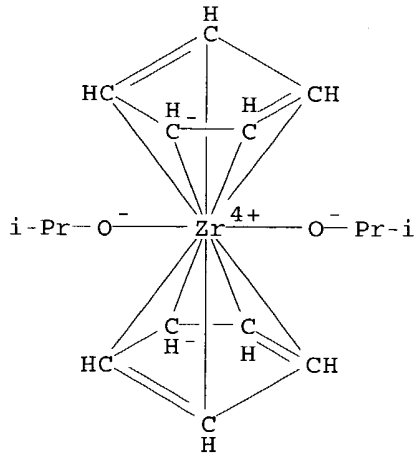
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(aldol condensation with furfural and hydride reduction of)
RN 67-64-1 HCAPLUS
CN 2-Propanone (9CI) (CA INDEX NAME)



IT **37342-98-6 78091-18-6**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalyst, for oxidation of allylic alcs.)
RN 37342-98-6 HCAPLUS
CN Zirconium, bis(η5-2,4-cyclopentadien-1-yl)dihydro- (9CI) (CA INDEX NAME)

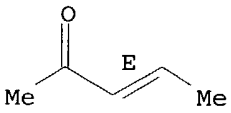


RN 78091-18-6 HCAPLUS
CN Zirconium, bis(η5-2,4-cyclopentadien-1-yl)bis(2-propanolato)- (9CI) (CA INDEX NAME)

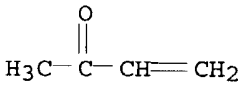


IT **3102-33-8P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
RN 3102-33-8 HCAPLUS
CN 3-Penten-2-one, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IT **78-94-4P**, preparation
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of, by oxidation of allylic alc., zirconocene complex-catalyzed)
RN 78-94-4 HCAPLUS
CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



L32 ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1987:554895 HCAPLUS
DOCUMENT NUMBER: 107:154895
TITLE: Catalytic oxidative dehydrogenation process
INVENTOR(S): Bajars, Laimonis; Croce, Louis J.
PATENT ASSIGNEE(S): Petro-Tex Chemical Corp., USA
SOURCE: U.S., 12 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4658074	A	19870414	US 1965-459878	19650528

PRIORITY APPLN. INFO.: US 1965-459878 19650528
OTHER SOURCE(S): CASREACT 107:154895

AB C1-12 organic compds. having ≥1C2H2 grouping are oxidatively dehydrogenated at ≥250° with ≥0.2 mol O per mol of organic compound in the presence of a ferrite catalyst having ≥1 metal selected from the group Cu,Al,Cr,Ti,V,Mo,W,Na,Li,K,Sn,Pb,Sb,Bi,Ga, and rare earth metals. The ferrite catalyst cations have an ionic radius of 0.5-1.1 Å, are present in a total amount of 0.05-2.0 atoms per atom Fe, and catalyst crystal structure is a face-centered cubic form. Thus, 15 mL EG-2 ($ZnFe_2O_4$) charged into a reactor and fed a mixture of O, steam, and MeCOCHMe2 (I), in an amount of 0.5 mol O per mol I, and 20 mol steam per mol I at 425° with LHSV feed rate 1.0 gave MeCOCMe:CH2.

IC ICM C07C005-48
ICS C07C005-50

NCL 585380000

CC 35-2 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 23, 25, 67

IT 7429-90-5, Aluminum, uses and miscellaneous 7439-92-1, Lead, uses and miscellaneous 7439-93-2, Lithium, uses and miscellaneous 7439-98-7, Molybdenum, uses and miscellaneous 7440-09-7, Potassium, uses and miscellaneous 7440-23-5, Sodium, uses and miscellaneous 7440-31-5, Tin, uses and miscellaneous **7440-32-6**, Titanium, uses and miscellaneous 7440-33-7, Tungsten, uses and miscellaneous 7440-36-0, Antimony, uses and miscellaneous 7440-47-3, Chromium, uses and miscellaneous 7440-48-4, uses and miscellaneous 7440-50-8, Copper, uses and miscellaneous 7440-55-3, Gallium, uses and miscellaneous 7440-62-2, Vanadium, uses and miscellaneous 7440-69-9, Bismuth, uses and miscellaneous 7553-56-2, Iodine, uses and miscellaneous 7723-14-0, Phosphorus, uses and miscellaneous 7782-50-5, Chlorine, uses and miscellaneous 10035-10-6, Hydrogen bromide, uses and miscellaneous
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, containing ferrites, for oxidative dehydrogenation of C1-12 organic compds.)

IT 11113-67-0 11138-11-7, Barium ferrite 12063-19-3, Zinc ferrite 12068-86-9, Magnesium ferrite 12612-43-0 12656-79-0 12737-27-8 37220-43-2 37367-93-4 **39361-81-4** 60063-27-6
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, for oxidative dehydrogenation of C1-12 organic compds.)

IT **814-78-8P**, Methyl isopropenyl ketone
RL: IMF (Industrial manufacture); **PREP (Preparation)**
(manufacture of, from methylbutanone, ferrite oxidative dehydrogenation catalysts for)

IT **547-63-7**, Methyl isobutyrate
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(oxidative dehydrogenation of, Me methacrylate from, ferrite catalysts for)

IT **123-38-6**, Propionaldehyde, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(oxidative dehydrogenation of, acrolein from, ferrite catalysts for)

IT **563-80-4**, Methyl isopropyl ketone
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(oxidative dehydrogenation of, methylbutenone from, ferrite catalysts for)

IT **7440-32-6**, Titanium, uses and miscellaneous
RL: **CAT (Catalyst use)**; USES (Uses)

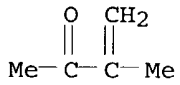
(catalysts, containing ferrites, for oxidative dehydrogenation of C1-12 organic compds.)
RN 7440-32-6 HCAPLUS
CN Titanium (8CI, 9CI) (CA INDEX NAME)

Ti

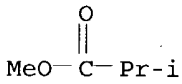
IT **39361-81-4**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, for oxidative dehydrogenation of C1-12 organic compds.)
RN 39361-81-4 HCAPLUS
CN Iron zirconium oxide (9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
O	x	17778-80-2
Zr	x	7440-67-7
Fe	x	7439-89-6

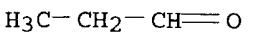
IT **814-78-8P**, Methyl isopropenyl ketone
RL: IMF (Industrial manufacture); **PREP (Preparation)**
(manufacture of, from methylbutanone, ferrite oxidative dehydrogenation catalysts for)
RN 814-78-8 HCAPLUS
CN 3-Buten-2-one, 3-methyl- (8CI, 9CI) (CA INDEX NAME)



IT **547-63-7**, Methyl isobutyrate
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(oxidative dehydrogenation of, Me methacrylate from, ferrite catalysts for)
RN 547-63-7 HCAPLUS
CN Propanoic acid, 2-methyl-, methyl ester (9CI) (CA INDEX NAME)

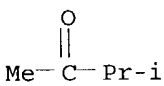


IT **123-38-6**, Propionaldehyde, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(oxidative dehydrogenation of, acrolein from, ferrite catalysts for)
RN 123-38-6 HCAPLUS
CN Propanal (9CI) (CA INDEX NAME)



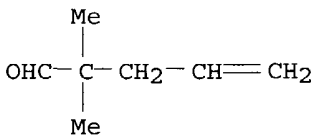
IT **563-80-4**, Methyl isopropyl ketone

RL: **RCT (Reactant); RACT (Reactant or reagent)**
(oxidative dehydrogenation of, methylbutenone from, ferrite catalysts for)
RN 563-80-4 HCAPLUS
CN 2-Butanone, 3-methyl- (8CI, 9CI) (CA INDEX NAME)

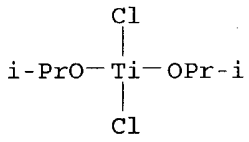


L32 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1986:571894 HCAPLUS
DOCUMENT NUMBER: 105:171894
TITLE: Silicon-mediated annulation. Part 2. A synthesis of β-alkoxy cyclooctanones via intramolecular directed aldol reactions
AUTHOR(S): Cockerill, G. Stuart; Kocienski, Philip; Treadgold, Richard
CORPORATE SOURCE: Dep. Org. Chem., Univ. Leeds, Leeds, LS2 9JT, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1985), (10), 2101-8
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 105:171894
AB β-Alkoxycyclooctanones were formed in poor to moderate yield by Lewis acid-catalyzed intramol. directed aldol reaction between an acetal and an enol silane. Thus, treatment enol silane I with 1.1 equiv TiCl4 in CH2Cl2 at -78° gave 56% benzocyclooctanone II after 15 min. The effect of chain substitution, Lewis acid, and acetal structure on the efficiency of 8-exo, endo-cyclization was discussed.
CC 24-6 (Alicyclic Compounds)
IT **5497-67-6**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(Grignard methylation or acetalization with ethylene glycol)
IT **762-99-2 20717-86-6** 27607-77-8
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, for intramol. aldol cyclization of acetal enol silanes)
IT **67-64-1**, reactions
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(condensation of, with di-Me pentenal)
IT 56037-91-3P **58143-79-6P** 104730-33-8P **104730-38-3P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation); RACT (Reactant or reagent)**
(preparation and oxidation of)
IT **83333-61-3P 101773-33-5P 104730-34-9P 104730-40-7P 104730-41-8P 104730-47-4P 104730-48-5P 104730-50-9P 104730-51-0P 104746-68-1P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and trimethylsilylation of)
IT **141-79-7**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(reaction of, with (chloropropyl)dioxolane)

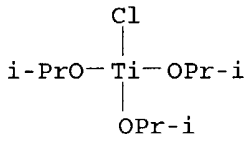
IT **5497-67-6**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(Grignard methylation or acetalization with ethylene glycol)
RN 5497-67-6 HCAPLUS
CN 4-Pentenal, 2,2-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



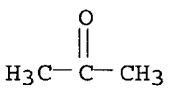
IT **762-99-2 20717-86-6**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, for intramol. aldol cyclization of acetal enol silanes)
RN 762-99-2 HCAPLUS
CN Titanium, dichlorobis(2-propanolato)-, (T-4)- (9CI) (CA INDEX NAME)



RN 20717-86-6 HCAPLUS
CN Titanium, chlorotris(2-propanolato)-, (T-4)- (9CI) (CA INDEX NAME)

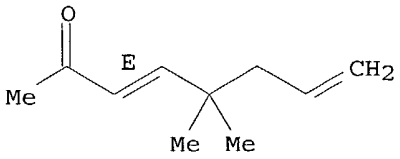


IT **67-64-1**, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(condensation of, with di-Me pentenal)
RN 67-64-1 HCAPLUS
CN 2-Propanone (9CI) (CA INDEX NAME)

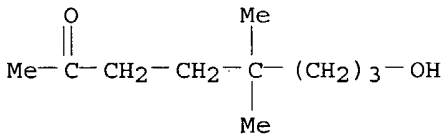


IT **58143-79-6P 104730-38-3P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; **RACT (Reactant or reagent)**
(preparation and oxidation of)
RN 58143-79-6 HCAPLUS
CN 3,7-Octadien-2-one, 5,5-dimethyl-, (E)- (9CI) (CA INDEX NAME)

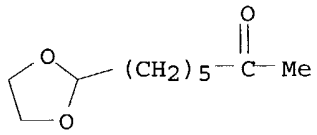
Double bond geometry as shown.



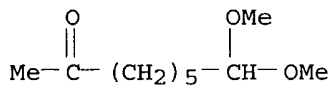
RN 104730-38-3 HCAPLUS
CN 2-Octanone, 8-hydroxy-5,5-dimethyl- (9CI) (CA INDEX NAME)



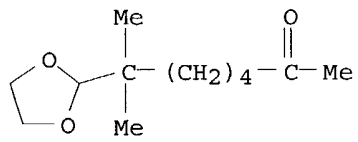
IT **83333-61-3P 101773-33-5P 104730-34-9P**
104730-40-7P 104730-41-8P 104730-47-4P
104730-48-5P 104730-50-9P 104730-51-0P
104746-68-1P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and trimethylsilylation of)
RN 83333-61-3 HCAPLUS
CN 2-Heptanone, 7-(1,3-dioxolan-2-yl)- (9CI) (CA INDEX NAME)



RN 101773-33-5 HCAPLUS
CN 2-Octanone, 8,8-dimethoxy- (9CI) (CA INDEX NAME)

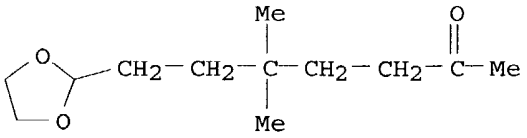


RN 104730-34-9 HCAPLUS
CN 2-Octanone, 7-(1,3-dioxolan-2-yl)-7-methyl- (9CI) (CA INDEX NAME)

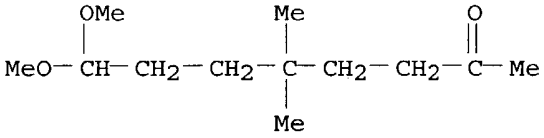


RN 104730-40-7 HCAPLUS

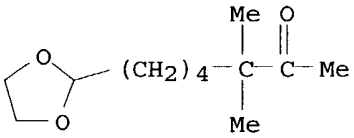
CN 2-Heptanone, 7-(1,3-dioxolan-2-yl)-5,5-dimethyl- (9CI) (CA INDEX NAME)



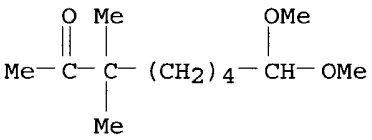
RN 104730-41-8 HCAPLUS
CN 2-Octanone, 8,8-dimethoxy-5,5-dimethyl- (9CI) (CA INDEX NAME)



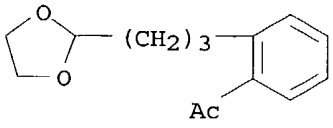
RN 104730-47-4 HCAPLUS
CN 2-Heptanone, 7-(1,3-dioxolan-2-yl)-3,3-dimethyl- (9CI) (CA INDEX NAME)



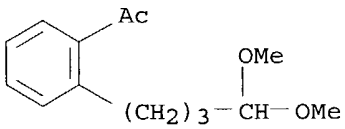
RN 104730-48-5 HCAPLUS
CN 2-Octanone, 8,8-dimethoxy-3,3-dimethyl- (9CI) (CA INDEX NAME)



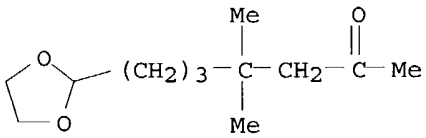
RN 104730-50-9 HCAPLUS
CN Ethanone, 1-[2-[3-(1,3-dioxolan-2-yl)propyl]phenyl]- (9CI) (CA INDEX NAME)



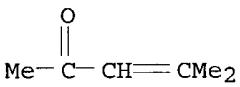
RN 104730-51-0 HCAPLUS
CN Ethanone, 1-[2-(4,4-dimethoxybutyl)phenyl]- (9CI) (CA INDEX NAME)



RN 104746-68-1 HCAPLUS
CN 2-Heptanone, 7-(1,3-dioxolan-2-yl)-4,4-dimethyl- (9CI) (CA INDEX NAME)



IT **141-79-7**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(reaction of, with (chloropropyl)dioxolane)
RN 141-79-7 HCAPLUS
CN 3-Penten-2-one, 4-methyl- (8CI, 9CI) (CA INDEX NAME)



L32 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1981:496967 HCAPLUS
DOCUMENT NUMBER: 95:96967
TITLE: Synthesis of methyl vinyl ketone from acetone and formaldehyde by the one-step condensation in vapor phase
AUTHOR(S): Igarashi, Tetsutaro; Suzuki, Michio
CORPORATE SOURCE: Dep. Chem. Technol., Kanagawa Univ., Yokohama, Japan
SOURCE: Kanagawa Daigaku Kogakubu Kenkyu Hokoku (1981), 19, 64-8
CODEN: KGDKBU; ISSN: 0368-5381
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
AB In the title synthesis the yield was 54% and the optimum conditions were: HCHO-Me2CO molar ratio 0.25, feed rate 0.58 g/g catalyst (Zr/SiO2)/min, and temperature 300°.
CC 23-15 (Aliphatic Compounds)
IT **7440-67-7**, uses and miscellaneous
RL: **CAT (Catalyst use)**; USES (Uses)
(catalyst, for condensation of acetone with formaldehyde)
IT **78-94-4P**, preparation
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of, by vapor phase condensation of acetone with formaldehyde, optimization of)
IT **50-00-0**, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(vapor-phase condensation of, with acetone, optimization of)
IT **67-64-1**, reactions

RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(vapor-phase condensation of, with formaldehyde, optimization of)

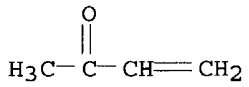
IT **7440-67-7**, uses and miscellaneous
RL: **CAT (Catalyst use)**; USES (Uses)
(catalyst, for condensation of acetone with formaldehyde)

RN 7440-67-7 HCAPLUS
CN Zirconium (8CI, 9CI) (CA INDEX NAME)

Zr

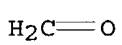
IT **78-94-4P**, preparation
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of, by vapor phase condensation of acetone with formaldehyde, optimization of)

RN 78-94-4 HCAPLUS
CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



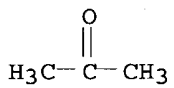
IT **50-00-0**, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(vapor-phase condensation of, with acetone, optimization of)

RN 50-00-0 HCAPLUS
CN Formaldehyde (8CI, 9CI) (CA INDEX NAME)



IT **67-64-1**, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(vapor-phase condensation of, with formaldehyde, optimization of)

RN 67-64-1 HCAPLUS
CN 2-Propanone (9CI) (CA INDEX NAME)



L32 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1974:426165 HCAPLUS
DOCUMENT NUMBER: 81:26165
TITLE: Vinyl monomers from formalin and aldehydes, ketones, esters, or nitriles
INVENTOR(S): Fukui, Masahiro; Ishibe, Tetsuya; Koga, Isao; Inoi, Takeshi
PATENT ASSIGNEE(S): Chisso Corp.
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent

LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 48078113	A2	19731020	JP 1972-9598	19720126
JP 57013531	B4	19820317		

PRIORITY APPLN. INFO.: JP 1972-9598 19720126

AB Vinyl monomers were prepared in the presence of a zirconium oxide [1314-23-4] catalyst. Thus, SiO2 was impregnated with aqueous Zr(NO3)4, dried, and heated at 500.deg. for 3 hr to give 10% ZrO2-SiO2. The catalyst was packed into a quartz tube and treated with 1:3 M 35% formaldehyde [50-00-0]-acetone [67-64-1] mixture at 300.deg. to give Me vinyl ketone [78-94-4] with 57% conversion and 93% selectivity. Also prepared were styrene [100-42-5], 2-ethyl-2-propenal [922-63-4], methacrylonitrile [126-98-7], and Me methacrylate [80-62-6].

NCL 16B52
CC 35-2 (Synthetic High Polymers)
Section cross-reference(s): 23

IT **1314-23-4**, uses and miscellaneous
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, for manufacture of vinyl monomers)

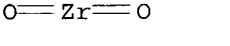
IT **78-94-4P** 80-62-6P 100-42-5P, preparation 126-98-7P
922-63-4P
RL: IMF (Industrial manufacture); **PREP (Preparation)**
(manufacture of, catalysts for)

IT **50-00-0**, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(with acetone, for Me vinyl ketone manufacture)

IT **67-64-1**, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(with formaldehyde, for Me vinyl ketone manufacture)

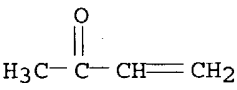
IT **1314-23-4**, uses and miscellaneous
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, for manufacture of vinyl monomers)

RN 1314-23-4 HCAPLUS
CN Zirconium oxide (ZrO2) (8CI, 9CI) (CA INDEX NAME)



IT **78-94-4P**
RL: IMF (Industrial manufacture); **PREP (Preparation)**
(manufacture of, catalysts for)

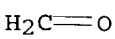
RN 78-94-4 HCAPLUS
CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



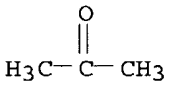
IT **50-00-0**, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(with acetone, for Me vinyl ketone manufacture)

RN 50-00-0 HCAPLUS

CN Formaldehyde (8CI, 9CI) (CA INDEX NAME)



IT **67-64-1**, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(with formaldehyde, for Me vinyl ketone manufacture)
RN 67-64-1 HCAPLUS
CN 2-Propanone (9CI) (CA INDEX NAME)



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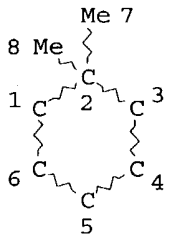
L12 STR

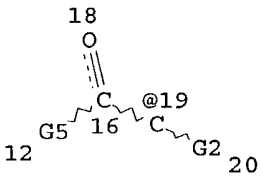


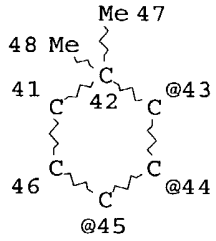
← gem-dimethyl C6 ring

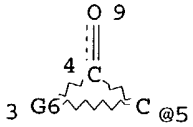
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

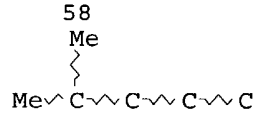
GRAPH ATTRIBUTES:
RSPEC 2
NUMBER OF NODES IS 8

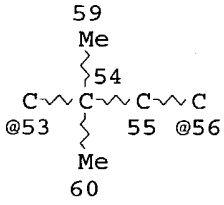
STEREO ATTRIBUTES: NONE
L16 STR











VAR G1=5/19
VAR G2=H/ME
VAR G4=CH2/39
VAR G5=43/44/45
VAR G6=49-4 52-5/52-4 49-5/53-4 56-5/56-4 53-5
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 33

STEREO ATTRIBUTES: NONE
L18 7978541 SEA FILE=REGISTRY ABB=ON PLU=ON C6/ES AND O/ELS AND NC=1 NOT

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                (PMS OR IDS)/CI AND NR<5 AND C>10
L20          398 SEA FILE=REGISTRY SUB=L18 SSS FUL L12 AND L16
L21          317 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20(L)PREP/RL
L28              TRANSFER  PLU=ON  L21 1- RN :    5326 TERMS
L29         5326 SEA FILE=REGISTRY ABB=ON  PLU=ON  L28
L30              STR
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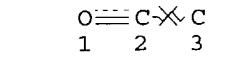

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1   2   3

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   3

STEREO ATTRIBUTES: NONE
L32         3515 SEA FILE=REGISTRY SUB=L29 SSS FUL L30
L33              STR
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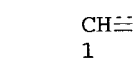

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1   2

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   2

STEREO ATTRIBUTES: NONE
L35          264 SEA FILE=REGISTRY SUB=L29 SSS FUL L33
L36       280202 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L32(L)(RACT OR RCT OR RGT)/RL

L37       114368 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L35(L)(RACT OR RCT OR RGT)/RL

L38        98133 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L36 AND L37
L39          111 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L38 AND L21
L40            4 SEA FILE=REGISTRY ABB=ON  PLU=ON  L29 AND (TI OR ZR OR HF)/ELS

L41            1 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L39 AND L40
L42           19 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L39 AND CATAL?
L43           18 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L42 NOT L41


=> d ibib ab hitind hitstr 1-18

L43  ANSWER 1 OF 18  HCAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:         2003:424482  HCAPLUS
DOCUMENT NUMBER:          139:7042
TITLE:                    Preparation of isomeric mixtures of cyclohexenyl
                          methyl ketone as intermediates for damascones
INVENTOR(S):              Yamamoto, Takeshi; Watabe, Shinya; Ujihara, Hideo;
                          Hagiwara, Toshimitsu
PATENT ASSIGNEE(S):       Takasago Perfumery Co., Ltd., Japan
SOURCE:                   Jpn. Kokai Tokkyo Koho, 8 pp.
```

CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003160529	A2	20030603	JP 2001-363575	20011129

PRIORITY APPLN. INFO.: JP 2001-363575 20011129

AB Mixts. of 2,2,6-trimethyl-5-cyclohexenyl Me ketone (I), 2,2,6-trimethyl-6-cyclohexenyl Me ketone (II), and 2,2,6-trimethyl-4-cyclohexenyl Me ketone (III) are prepared by isomerization of III in the presence of **catalysts**. Isomeric mixts. of damascone, useful as fragrances, are prepared by reaction of the I-II-III mixts. with MeCHO and dehydration with acids. Cis-III (preparation given) was heated in tetraethylene glycol monomethyl ether in the presence of t-BuOK at 175° for 4 h to give a composition comprising III (cis/trans = 2/98) 12, I 61, and II 27%, which was converted into a composition comprising δ-damascone 11, α-damascone 63.5, and β-damascone 25.5%.

IC ICM C07C045-67
ICS C07C049-543; C07C403-14; C07B061-00

CC 30-10 (Terpenes and Terpenoids)
Section cross-reference(s): 62

IT Metal alkoxides
RL: CAT (Catalyst use); USES (Uses)
(alkali metal, isomerization **catalysts**; preparation of isomeric mixts. of cyclohexenyl Me ketone as intermediates for fragrant damascones)

IT Alkali metal compounds
RL: CAT (Catalyst use); USES (Uses)
(alkoxides, isomerization **catalysts**; preparation of isomeric mixts. of cyclohexenyl Me ketone as intermediates for fragrant damascones)

IT Transition metal chlorides
RL: CAT (Catalyst use); USES (Uses)
(isomerization **catalysts**; preparation of isomeric mixts. of cyclohexenyl Me ketone as intermediates for fragrant damascones)

IT Isomerization **catalysts**
Perfumes
(preparation of isomeric mixts. of cyclohexenyl Me ketone as intermediates for fragrant damascones)

IT 865-47-4, tert-Butoxypotassium 13569-65-8, Rhodium trichloride trihydrate
RL: CAT (Catalyst use); USES (Uses)
(isomerization **catalysts**; preparation of isomeric mixts. of cyclohexenyl Me ketone as intermediates for fragrant damascones)

IT **35044-68-9P 43052-87-5P**, α-Damascone
535933-86-9P 535933-88-1P, trans-δ-Damascone
RL: COS (Cosmetic use); IMF (Industrial manufacture); SPN (Synthetic preparation); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of isomeric mixts. of cyclohexenyl Me ketone as intermediates for fragrant damascones)

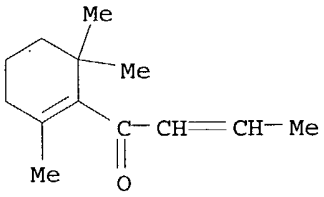
IT **1197-92-8P 37709-66-3P 41435-93-2P 41436-48-0P**
RL: IMF (Industrial manufacture); **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation of isomeric mixts. of cyclohexenyl Me ketone as intermediates

for fragrant damascones)

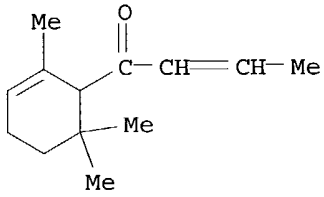
IT **75-07-0**, Acetaldehyde, reactions **141-79-7**, Mesityl oxide
504-60-9, 1,3-Pentadiene
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(preparation of isomeric mixts. of cyclohexenyl Me ketone as intermediates for fragrant damascones)

IT **35044-68-9P 43052-87-5P**, α-Damascone
535933-86-9P 535933-88-1P, trans-δ-Damascone
RL: COS (Cosmetic use); IMF (Industrial manufacture); SPN (Synthetic preparation); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of isomeric mixts. of cyclohexenyl Me ketone as intermediates for fragrant damascones)

RN 35044-68-9 HCAPLUS
CN 2-Buten-1-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)

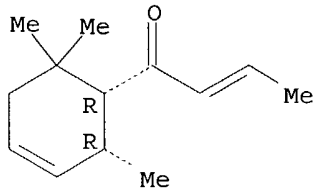


RN 43052-87-5 HCAPLUS
CN 2-Buten-1-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



RN 535933-86-9 HCAPLUS
CN 2-Buten-1-one, 1-[(1R,2R)-2,6,6-trimethyl-3-cyclohexen-1-yl]-, rel- (9CI) (CA INDEX NAME)

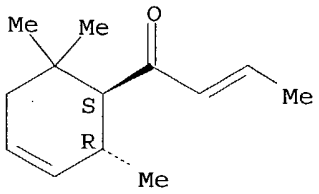
Relative stereochemistry.
Double bond geometry unknown.



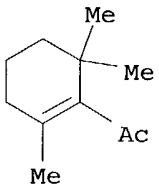
RN 535933-88-1 HCAPLUS
CN 2-Buten-1-one, 1-[(1R,2S)-2,6,6-trimethyl-3-cyclohexen-1-yl]-, rel- (9CI)

(CA INDEX NAME)

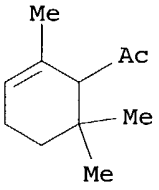
Relative stereochemistry.
Double bond geometry unknown.



IT **1197-92-8P 37709-66-3P 41435-93-2P**
41436-48-0P
RL: IMF (Industrial manufacture); **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation of isomeric mixts. of cyclohexenyl Me ketone as intermediates for fragrant damascones)
RN 1197-92-8 HCAPLUS
CN Ethanone, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)

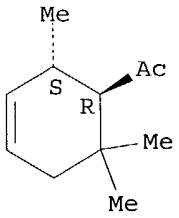


RN 37709-66-3 HCAPLUS
CN Ethanone, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



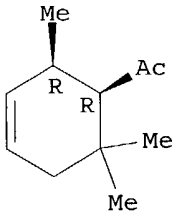
RN 41435-93-2 HCAPLUS
CN Ethanone, 1-[(1R,2S)-2,6,6-trimethyl-3-cyclohexen-1-yl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 41436-48-0 HCAPLUS
CN Ethanone, 1-[(1R,2R)-2,6,6-trimethyl-3-cyclohexen-1-yl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT **75-07-0**, Acetaldehyde, reactions **141-79-7**, Mesityl oxide
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(preparation of isomeric mixts. of cyclohexenyl Me ketone as intermediates for fragrant damascones)
RN 75-07-0 HCAPLUS
CN Acetaldehyde (8CI, 9CI) (CA INDEX NAME)

$H_3C-CH=O$

RN 141-79-7 HCAPLUS
CN 3-Penten-2-one, 4-methyl- (8CI, 9CI) (CA INDEX NAME)

$Me-C(=O)-CH=CMe_2$

L43 ANSWER 2 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:247917 HCAPLUS
DOCUMENT NUMBER: 138:401925
TITLE: Synthesis of CDE and BCDE Molecular Fragments of the Limonoids Havanensin and Azadiradione
AUTHOR(S): Fernandez-Mateos, A.; Mateos Buron, L.; Martin de la Nava, E. M.; Rubio Gonzalez, R.
CORPORATE SOURCE: Facultad de C. Quimicas, Departamento de Quimica Organica, Universidad de Salamanca, Salamanca, 37008, Spain
SOURCE: Journal of Organic Chemistry (2003), 68(9), 3585-3592
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:401925

AB A new approach to the synthesis of CDE and BCDE mol. fragments, such as I and II, of the limonoids havanensin and azadiradione has been achieved from cyclocitral and drimenal in seven steps in overall yields of 20 and 9%, resp.

CC 30-30 (Terpenes and Terpenoids)
Section cross-reference(s): 75

IT Addition reaction
(conjugate; of diphenylzinc to an enone **catalyzed** by Ni(II) in preparation of CDE and BCDE mol. fragments of havanensin and azadiradione)

IT **531512-85-3P**
RL: PRP (Properties); **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(crystal structure; preparation of CDE and BCDE mol. fragments of havanensin and azadiradione)

IT **108-24-7**, Acetic anhydride
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(for electrocyclization in preparation of CDE and BCDE mol. fragments of havanensin and azadiradione)

IT **531512-81-9P 531512-86-4P 531512-96-6P**
RL: PRP (Properties); **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation of CDE and BCDE mol. fragments of havanensin and azadiradione)

IT 108-86-1, Bromobenzene, reactions **432-25-7**, β-Cyclocitral 1826-67-1, Vinylmagnesium bromide **148615-75-2**, (±)-Drimenal
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(preparation of CDE and BCDE mol. fragments of havanensin and azadiradione)

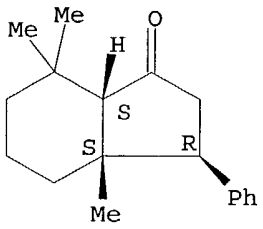
IT 51768-87-7P **56248-16-9P 83113-64-8P**, (±)-β-Drimenal **531512-76-2P** 531512-79-5P **531512-80-8P** 531512-87-5P 531512-89-7P 531512-92-2P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; **RACT (Reactant or reagent)**
(preparation of CDE and BCDE mol. fragments of havanensin and azadiradione)

IT **531512-85-3P**
RL: PRP (Properties); **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(crystal structure; preparation of CDE and BCDE mol. fragments of havanensin and azadiradione)

RN 531512-85-3 HCAPLUS

CN 1H-Inden-1-one, octahydro-3a,7,7-trimethyl-3-phenyl-, (3R,3aS,7aS)-rel- (9CI) (CA INDEX NAME)

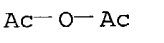
Relative stereochemistry.



IT **108-24-7**, Acetic anhydride

RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(for electrocyclization in preparation of CDE and BCDE mol. fragments of havanensin and azadiradione)

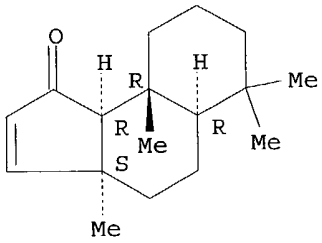
RN 108-24-7 HCAPLUS
CN Acetic acid, anhydride (9CI) (CA INDEX NAME)



IT **531512-81-9P 531512-86-4P 531512-96-6P**
RL: PRP (Properties); **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation of CDE and BCDE mol. fragments of havanensin and azadiradione)

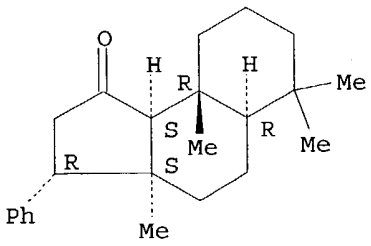
RN 531512-81-9 HCAPLUS
CN 1H-Benz[e]inden-1-one, 3a,4,5,5a,6,7,8,9,9a,9b-decahydro-3a,6,6,9a-tetramethyl-, (3aR,5aS,9aS,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



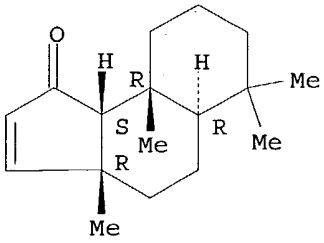
RN 531512-86-4 HCAPLUS
CN 1H-Benz[e]inden-1-one, dodecahydro-3a,6,6,9a-tetramethyl-3-phenyl-, (3R,3aS,5aR,9aR,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

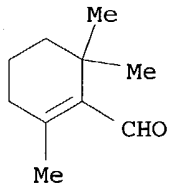


RN 531512-96-6 HCAPLUS
CN 1H-Benz[e]inden-1-one, 3a,4,5,5a,6,7,8,9,9a,9b-decahydro-3a,6,6,9a-tetramethyl-, (3aR,5aR,9aR,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

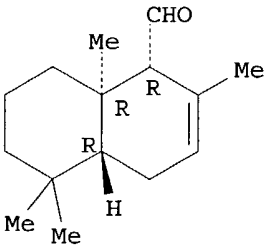


IT **432-25-7**, β-Cyclocitral **148615-75-2**,
(±)-Drimenal
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(preparation of CDE and BCDE mol. fragments of havanensin and azadiradione)
RN 432-25-7 HCAPLUS
CN 1-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

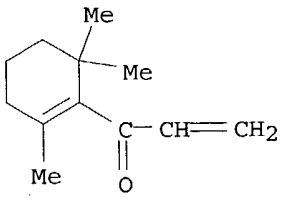


RN 148615-75-2 HCAPLUS
CN 1-Naphthalenecarboxaldehyde, 1,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-, (1R,4aR,8aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

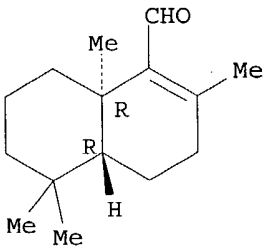


IT **56248-16-9P 83113-64-8P**, (±)-β-Drimenal
531512-76-2P 531512-80-8P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; **RACT (Reactant or reagent)**
(preparation of CDE and BCDE mol. fragments of havanensin and azadiradione)
RN 56248-16-9 HCAPLUS
CN 2-Propen-1-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



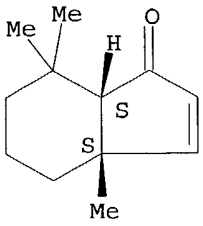
RN 83113-64-8 HCAPLUS
CN 1-Naphthalenecarboxaldehyde, 3,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-, (4aR,8aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



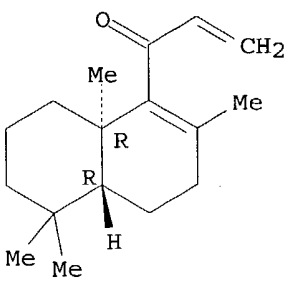
RN 531512-76-2 HCAPLUS
CN 1H-Inden-1-one, 3a,4,5,6,7,7a-hexahydro-3a,7,7-trimethyl-, (3aR,7aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 531512-80-8 HCAPLUS
CN 2-Propen-1-one, 1-[(4aR,8aR)-3,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-1-naphthalenyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L43 ANSWER 3 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:900120 HCAPLUS
DOCUMENT NUMBER: 136:20169
TITLE: Process for production of cyclohexenyl methyl ketones as intermediates for perfumery damascones
INVENTOR(S): Watanabe, Shinya; Ujihara, Hideo; Yamamoto, Takeshi; Hagiwara, Toshimitsu
PATENT ASSIGNEE(S): Takasago International Corporation, Japan
SOURCE: Eur. Pat. Appl., 12 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1162190	A2	20011212	EP 2001-401471	20010607
EP 1162190	A3	20020130		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2001348355	A2	20011218	JP 2000-170823	20000607
US 2002004615	A1	20020110	US 2001-875158	20010607

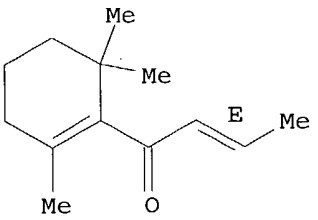
PRIORITY APPLN. INFO.: JP 2000-170823 A 20000607
OTHER SOURCE(S): CASREACT 136:20169; MARPAT 136:20169

AB An economical process for producing (2- and/or 1-)cyclohexenyl Me ketones which are intermediates for the synthesis of α- or β-damascone. In the presence of a **catalyst**, a 3-cyclohexenyl Me ketone (I) (R1, R2 and R3 each independently = H, Me and at least two of R1, R2 and R3 = Me), is isomerized.

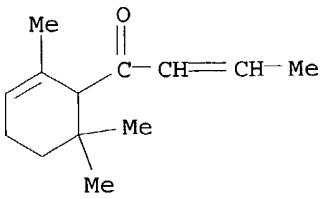
IC ICM C07C045-67
ICS C07C049-543
CC 30-10 (Terpenes and Terpenoids)
Section cross-reference(s): 62, 67
ST cyclohexenyl Me ketone isomerization **catalytic**; damascone perfumery intermediate process
IT Isomerization **catalysts**
(in production of cyclohexenyl Me ketones as intermediates for perfumery damascones)
IT **23726-91-2P**, β-Damascone **43052-87-5P**, α-Damascone
RL: COS (Cosmetic use); IMF (Industrial manufacture); SPN (Synthetic preparation); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(process for production of cyclohexenyl Me ketones as intermediates for perfumery damascones)
IT **1197-92-8P 37709-66-3P 41436-48-0P**
RL: IMF (Industrial manufacture); **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(process for production of cyclohexenyl Me ketones as intermediates for perfumery damascones)
IT **75-07-0**, Acetaldehyde, reactions **141-79-7**, Mesityl oxide 504-60-9, 1,3-Pentadiene
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(process for production of cyclohexenyl Me ketones as intermediates for perfumery damascones)

IT **23726-91-2P**, β-Damascone **43052-87-5P**, α-Damascone
RL: COS (Cosmetic use); IMF (Industrial manufacture); SPN (Synthetic preparation); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(process for production of cyclohexenyl Me ketones as intermediates for perfumery damascones)
RN 23726-91-2 HCAPLUS
CN 2-Buten-1-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (2E)- (9CI) (CA INDEX NAME)

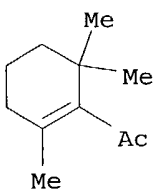
Double bond geometry as shown.



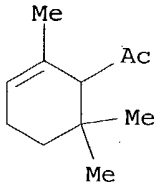
RN 43052-87-5 HCAPLUS
CN 2-Buten-1-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



IT **1197-92-8P 37709-66-3P 41436-48-0P**
RL: IMF (Industrial manufacture); **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(process for production of cyclohexenyl Me ketones as intermediates for perfumery damascones)
RN 1197-92-8 HCAPLUS
CN Ethanone, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)

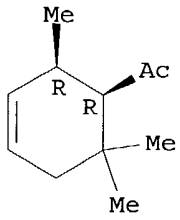


RN 37709-66-3 HCAPLUS
CN Ethanone, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)

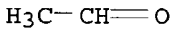


RN 41436-48-0 HCAPLUS
CN Ethanone, 1-[(1R,2R)-2,6,6-trimethyl-3-cyclohexen-1-yl]-, rel- (9CI) (CA INDEX NAME)

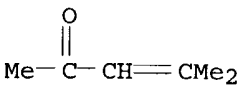
Relative stereochemistry.



IT **75-07-0**, Acetaldehyde, reactions **141-79-7**, Mesityl oxide
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(process for production of cyclohexenyl Me ketones as intermediates for perfumery damascones)
RN 75-07-0 HCAPLUS
CN Acetaldehyde (8CI, 9CI) (CA INDEX NAME)



RN 141-79-7 HCAPLUS
CN 3-Penten-2-one, 4-methyl- (8CI, 9CI) (CA INDEX NAME)



L43 ANSWER 4 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:664522 HCAPLUS
DOCUMENT NUMBER: 135:242372
TITLE: Method for preparation of damascone or damascenone by simultaneous **catalytic** oxidation and reduction of damascol and damascenol
INVENTOR(S): Watanabe, Kazunori
PATENT ASSIGNEE(S): Nippon Zeon Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001247504	A2	20010911	JP 2000-60171	20000306

PRIORITY APPLN. INFO.: JP 2000-60171 20000306
OTHER SOURCE(S): CASREACT 135:242372; MARPAT 135:242372

AB α, β, γ-Damascone and damascenone [I; wherein the dotted lines represent (1) one carbon-carbon double is present at 1, 2, or 3-position of the six-membered ring which possesses Me group at 2-position; (2) no carbon-carbon double bond is present in the six-membered ring which possesses Me group at 2-position; (3) two carbon-carbon double bonds are present at 1 and 3 or 2 and 4 positions in the six -membered ring which possesses Me group at 2-position; and (4) one carbon-carbon double bond is present in the six-membered ring which possesses Me group at 2-position] are prepared by contacting dehydro-α, β, γ-damascol and damascenol (II; wherein the dotted lines are defined as above) with a palladium complex **catalyst**. This process eliminates sep. oxidation and reduction steps of prior art methods and gives in short steps damascone or damascenone I which possess fruit or flower-like fragrance or taste and are useful as flavoring materials for food or cosmetics. Thus, 100 mg dehydro-β-damascol, which was prepared from β-cyclocitral, was dissolved in 2 mL PhMe, treated with 5 mol% Pd(OAc)2 and 35 mol% Ph3P, and stirred at 80° for 5 h to give 49% β-damascone.

IC ICM C07C045-29
ICS B01J031-24; C07C049-21; C07B061-00

CC 30-10 (Terpenes and Terpenoids)
Section cross-reference(s): 17, 63

ST damascone damascenone prepn flavoring material; palladium complex oxidn redn **catalyst**; damascol damascenol; simultaneous **catalytic** oxidn redn

IT Flavoring materials
Hydrogenation
Hydrogenation **catalysts**
Oxidation
Oxidation **catalysts**
(preparation of damascone or damascenone by simultaneous **catalytic** oxidation and reduction of damascol and damascenol)

IT Monoterpenes
RL: BUU (Biological use, unclassified); FFD (Food or feed use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of damascone or damascenone by simultaneous **catalytic** oxidation and reduction of damascol and damascenol)

IT **23726-91-2P**, β-Damascone **23726-93-4P**, β-Damascenone **24720-09-0P 41641-03-6P** **41641-04-7P 43052-87-5P**, α-Damascone **359865-01-3P 359865-02-4P**
RL: BUU (Biological use, unclassified); FFD (Food or feed use); SPN (Synthetic preparation); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of damascone or damascenone by simultaneous **catalytic** oxidation and reduction of damascol and damascenol)

IT 603-35-0, Triphenylphosphine, uses 3375-31-3
RL: CAT (Catalyst use); USES (Uses)
(preparation of damascone or damascenone by simultaneous **catalytic** oxidation and reduction of damascol and damascenol)

IT **116-26-7**, Safranal **432-25-7**, β-Cyclocitral

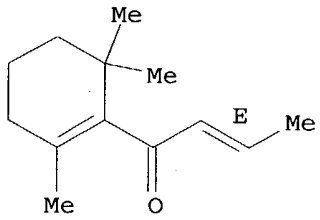
17522-32-6 359864-97-4 359864-98-5 359864-99-6 359865-00-2
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(preparation of damascone or damascenone by simultaneous **catalytic** oxidation and reduction of damascol and damascenol)

IT 23696-89-1P 359864-96-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of damascone or damascenone by simultaneous **catalytic** oxidation and reduction of damascol and damascenol)

IT **23726-91-2P**, β-Damascone **23726-93-4P**, β-Damascenone **24720-09-0P 41641-03-6P 41641-04-7P 43052-87-5P**, α-Damascone **359865-01-3P 359865-02-4P**
RL: BUU (Biological use, unclassified); FFD (Food or feed use); SPN (Synthetic preparation); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of damascone or damascenone by simultaneous **catalytic** oxidation and reduction of damascol and damascenol)

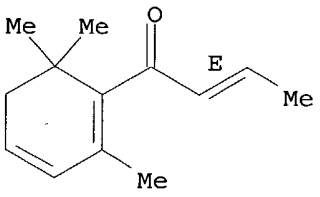
RN 23726-91-2 HCAPLUS
CN 2-Buten-1-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



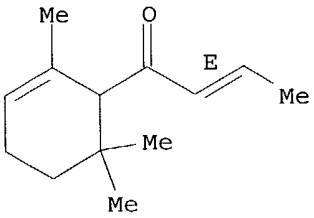
RN 23726-93-4 HCAPLUS
CN 2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



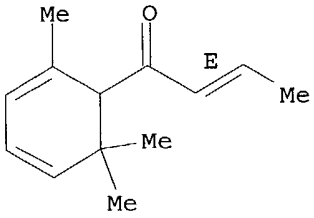
RN 24720-09-0 HCAPLUS
CN 2-Buten-1-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



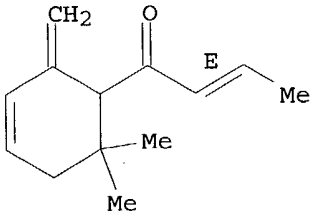
RN 41641-03-6 HCAPLUS
CN 2-Buten-1-one, 1-(2,6,6-trimethyl-2,4-cyclohexadien-1-yl)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

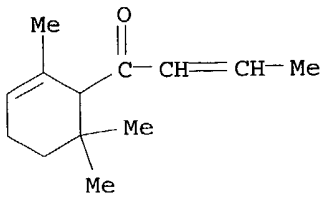


RN 41641-04-7 HCAPLUS
CN 2-Buten-1-one, 1-(6,6-dimethyl-2-methylene-3-cyclohexen-1-yl)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

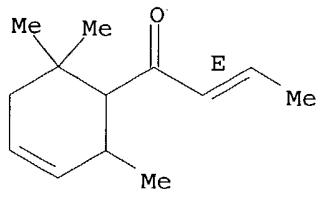


RN 43052-87-5 HCAPLUS
CN 2-Buten-1-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



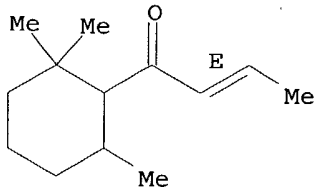
RN 359865-01-3 HCAPLUS
CN 2-Buten-1-one, 1-(2,6,6-trimethyl-3-cyclohexen-1-yl)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

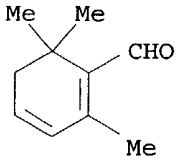


RN 359865-02-4 HCAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, (2E)- (9CI) (CA INDEX NAME)

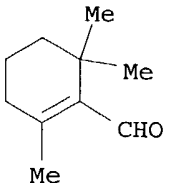
Double bond geometry as shown.



IT **116-26-7**, Safranal **432-25-7**, β-Cyclocitral
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(preparation of damascone or damascenone by simultaneous **catalytic** oxidation and reduction of damascol and damascenol)
RN 116-26-7 HCAPLUS
CN 1,3-Cyclohexadiene-1-carboxaldehyde, 2,6,6-trimethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 432-25-7 HCAPLUS
CN 1-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L43 ANSWER 5 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:282683 HCAPLUS
DOCUMENT NUMBER: 130:281783
TITLE: Method for synthesizing dihydroturkone
INVENTOR(S): He, Chengyao; Ding, Dalin; Li, Meirong; Hu, Yuanwen; Xiao, Hongwei; Wang, Zhigang; Zhang, Song; Wang, Shouyuan
PATENT ASSIGNEE(S): Yunan Prov. Chemical Industry Inst., Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 6 pp.
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

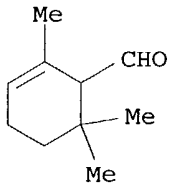
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1172099	A	19980204	CN 1997-105165	19970708
CN 1055078	B	20000802		

PRIORITY APPLN. INFO.: CN 1997-105165 19970708
OTHER SOURCE(S): CASREACT 130:281783

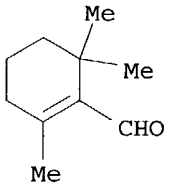
AB Dihydroturkone is prepared by **catalytic** addition reaction of cyclocitral and allyl halide (chloride, bromide) (cyclocitral-allyl halide ratio 1:0.95-2) at 60-80° with Sn or Zn powder as **catalyst** and benzene, toluene, or tetrafuran as solvent, oxidizing at 15-30° in acetone, benzene, toluene, tetrafuran, or DMF with pyridine chromate or CrO3 as oxidizing agent, and isomerization at 65-90° in benzene or toluene with K tert-butoxide or toluene-p-sulfonic acid as **catalyst**.

No

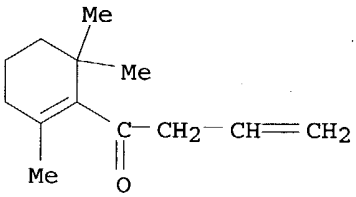
IC ICM C07C049-543
ICS C07C045-27; C07C045-61; C07C045-67
CC 24-5 (Alicyclic Compounds)
Section cross-reference(s): 30
IT 106-95-6, Allyl bromide, reactions 107-05-1, Allyl chloride **432-24-6**, α-Cyclocitral **432-25-7**, β-Cyclocitral
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(method for synthesizing dihydroturkone)
IT 28897-21-4P 28897-23-6P **31089-73-3P 31089-90-4P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(method for synthesizing dihydroturkone)
IT **35044-68-9P 43052-87-5P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(method for synthesizing dihydroturkone)
IT **432-24-6**, α-Cyclocitral **432-25-7**, β-Cyclocitral
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(method for synthesizing dihydroturkone)
RN 432-24-6 HCAPLUS
CN 2-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



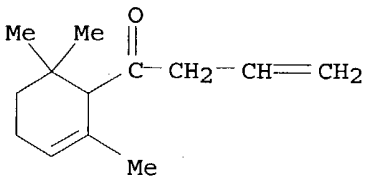
RN 432-25-7 HCAPLUS
CN 1-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **31089-73-3P 31089-90-4P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(method for synthesizing dihydroturkone)
RN 31089-73-3 HCAPLUS
CN 3-Buten-1-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)- (8CI, 9CI) (CA INDEX NAME)

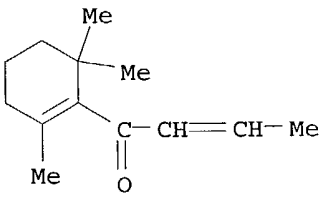


RN 31089-90-4 HCAPLUS
CN 3-Buten-1-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- (8CI, 9CI) (CA INDEX NAME)

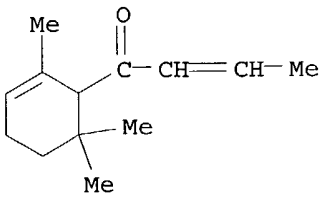


IT **35044-68-9P 43052-87-5P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(method for synthesizing dihydroturkone)
RN 35044-68-9 HCAPLUS

CN 2-Buten-1-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



RN 43052-87-5 HCAPLUS
CN 2-Buten-1-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)

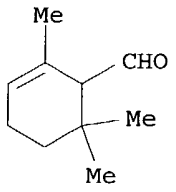


L43 ANSWER 6 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1994:557894 HCAPLUS
DOCUMENT NUMBER: 121:157894
TITLE: A new synthetic route to α-damascone
AUTHOR(S): Zheng, Ailian; Wu, Yuanlia
CORPORATE SOURCE: Inst. Mater. Med., Chin. Acad. Med. Sci., Beijing, 100050, Peop. Rep. China
SOURCE: Chinese Chemical Letters (1992), 3(3), 177-8
CODEN: CCLEE7; ISSN: 1001-8417
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 121:157894

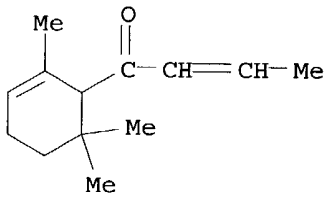
AB A new synthetic route to α-damascone (I) starting from citral is described. The synthesis features allylation of α-cyclocitral (1) with allyl bromide in the presence of tin powder to give the crucial intermediate diastereomeric butenols II in a combined yield of 70%; subsequent oxidation by pyridinium dichromate and rearrangement by TsOH gave I in a 51% overall yield.

CC 30-15 (Terpenes and Terpenoids)
ST alpha damascone; cyclocitral allylation tin **catalyst**
IT Allylation
(of α-cyclocitral by allyl bromide **catalyzed** by tin, α-damascone from)
IT 106-95-6, Allyl bromide, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(allylation by, of α-cyclocitral **catalyzed** by tin)
IT **432-24-6**, α-Cyclocitral
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(allylation of, by allyl bromide **catalyzed** by tin)
IT **43052-87-5P**, α-Damascone
RL: SPN (Synthetic preparation); **PREP (Preparation)**

(novel synthesis of)
IT 31089-90-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and acid-**catalyzed** rearrangement of, α-damascone from)
IT **432-24-6**, α-Cyclocitral
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(allylation of, by allyl bromide **catalyzed** by tin)
RN 432-24-6 HCAPLUS
CN 2-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **43052-87-5P**, α-Damascone
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(novel synthesis of)
RN 43052-87-5 HCAPLUS
CN 2-Buten-1-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



L43 ANSWER 7 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:102429 HCAPLUS
DOCUMENT NUMBER: 114:102429
TITLE: Photochemical syntheses of β-damascenone and β-damascone
AUTHOR(S): Wu, Guosheng; Hu, Jun; Wu, Biqi; Chen, Zhaobin; Wang, Yinzhang
CORPORATE SOURCE: Shanghai Inst. Org. Chem., Acad. Sin., Shanghai, Peop. Rep. China
SOURCE: Huaxue Xuebao (1990), 48(11), 1113-19
CODEN: HHHPA4; ISSN: 0567-7351
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
OTHER SOURCE(S): CASREACT 114:102429
AB β-Damascenone (I) and β-damascone (II) were synthesized from the same intermediate, the bisepoxide III, derived from the photooxidn. of allylic β-cyclogeraniol. Protection of the carbonyl group of III with o-nitrophenyl glycol, reduction, photodeprotection and dehydration gave II while I was obtained by means of acid **catalytic** ring-opening

of the epoxy groups of III, protection, reduction and photodeprotection. It was the first time to observe epoxidn. of terminal double bond under photooxidn.

CC 30-15 (Terpenes and Terpenoids)

IT **141-27-5**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(cyclization of)

IT **23726-91-2P**, β-Damascone **23726-93-4P**, β-Damascenone
RL: **RCT (Reactant)**; **PREP (Preparation)**; **RACT (Reactant or reagent)**
(photochem. synthesis of)

IT **432-25-7P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and Grignard reaction of, with Pr bromide)

IT **132367-14-7P 132367-15-8P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and dehydration of)

IT **432-24-6P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and isomerization of)

IT **132367-08-9P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; **RACT (Reactant or reagent)**
(preparation and ketalization of)

IT **132367-07-8P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation and phenylsulfonylation of)

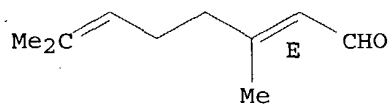
IT **132367-06-7P** 132367-11-4P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and ring cleavage of)

IT **141-27-5**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(cyclization of)

RN 141-27-5 HCAPLUS

CN 2,6-Octadienal, 3,7-dimethyl-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

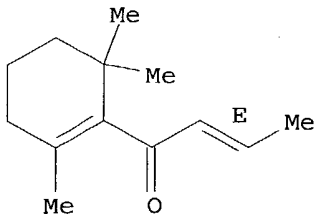


IT **23726-91-2P**, β-Damascone **23726-93-4P**, β-Damascenone
RL: **RCT (Reactant)**; **PREP (Preparation)**; **RACT (Reactant or reagent)**
(photochem. synthesis of)

RN 23726-91-2 HCAPLUS

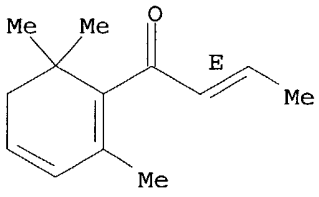
CN 2-Buten-1-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

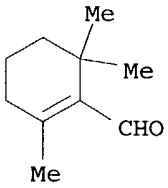


RN 23726-93-4 HCAPLUS
CN 2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (2E)- (9CI) (CA INDEX NAME)

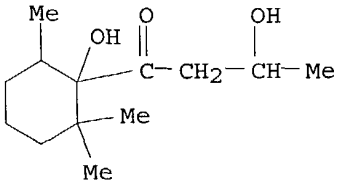
Double bond geometry as shown.



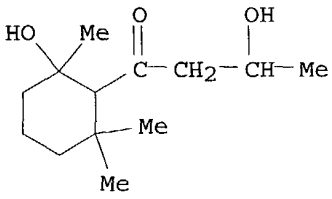
IT **432-25-7P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and Grignard reaction of, with Pr bromide)
RN 432-25-7 HCAPLUS
CN 1-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



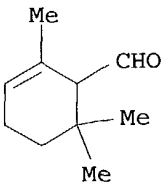
IT **132367-14-7P 132367-15-8P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and dehydration of)
RN 132367-14-7 HCAPLUS
CN 1-Butanone, 3-hydroxy-1-(1-hydroxy-2,2,6-trimethylcyclohexyl)- (9CI) (CA INDEX NAME)



RN 132367-15-8 HCAPLUS
CN 1-Butanone, 3-hydroxy-1-(2-hydroxy-2,6,6-trimethylcyclohexyl)- (9CI) (CA INDEX NAME)

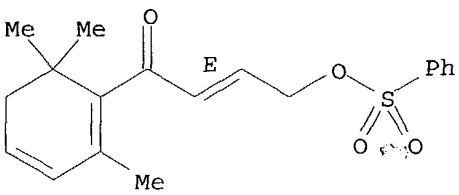


IT **432-24-6P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and isomerization of)
RN 432-24-6 HCAPLUS
CN 2-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



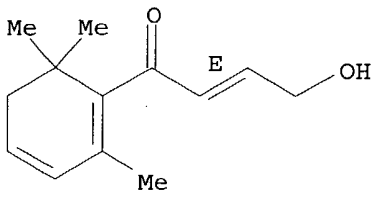
IT **132367-08-9P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; **RACT (Reactant or reagent)**
(preparation and ketalization of)
RN 132367-08-9 HCAPLUS
CN 2-Buten-1-one, 4-[(phenylsulfonyl)oxy]-1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

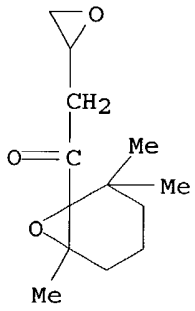


IT **132367-07-8P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation and phenylsulfonylation of)
RN 132367-07-8 HCAPLUS
CN 2-Buten-1-one, 4-hydroxy-1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (E)-
(9CI) (CA INDEX NAME)

Double bond geometry as shown.



IT **132367-06-7P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP
(Preparation); **RACT (Reactant or reagent)**
(preparation and ring cleavage of)
RN 132367-06-7 HCAPLUS
CN Ethanone, 2-oxiranyl-1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-
(9CI) (CA INDEX NAME)



L43 ANSWER 8 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1990:515592 HCAPLUS
DOCUMENT NUMBER: 113:115592
TITLE: Synthesis of α-damascone and 1-(2,6,6-trimethyl-2-tetrahydropyranyl)-2-alken-1-ones
AUTHOR(S): Erman, M. B.; Pribytkova, I. M.; Gulyi, S. I.; Bogomolova, O. A.; Cherkaev, G. V.; Aul'chenko, I. S.; Mochalin, V. B.
CORPORATE SOURCE: USSR
SOURCE: Zhurnal Organicheskoi Khimii (1989), 25(12), 2557-65
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 113:115592
AB α-Damascone (I) was prepared from α-cyclocitral by allylation with allyl bromide, oxidation of the resulting alc. by chromic acid, and rearrangement by Et3N. An analogous synthesis of β-damascone from 1-(4,6,6-trimethyl-1,3-cyclohexadienyl)-2-buten-1-one was unsuccessful

because of complications in the oxidation step. **Catalytic** (polyvanadylorganosiloxane) rearrangement of acetylenic alcs., e.g. II (R1 = H, R2 = Me, Et; R1 = R2 = Me) gave 1-(2,6,6-trimethyl-2-tetrahydropyranyl)-2-alken-1-ones.

CC 30-15 (Terpenes and Terpenoids)

IT **67-64-1**, Acetone, reactions **75-07-0**, Acetaldehyde, reactions **123-38-6**, Propionaldehyde, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(Grignard reaction of, with ethylmagnesium bromide and acetylenic alcs. and ethynyltrimethyltetrahydropyrans)

IT **432-24-6**, α-Cyclocitral **432-25-7** **41793-01-5**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(allylation of, by allyl bromide)

IT 127897-41-0P 127897-42-1P 127897-43-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and **catalytic** dehydrogenation-oxidation of)

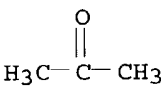
IT **127897-51-2P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and cyclization of)

IT 1719-19-3P 5876-76-6P **127897-50-1P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and dehydrogenation-oxidation of)

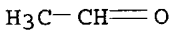
IT **43052-87-5P**, α-Damascone
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of, from α-cyclocitral)

IT **67-64-1**, Acetone, reactions **75-07-0**, Acetaldehyde, reactions **123-38-6**, Propionaldehyde, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(Grignard reaction of, with ethylmagnesium bromide and acetylenic alcs. and ethynyltrimethyltetrahydropyrans)

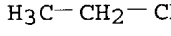
RN 67-64-1 HCAPLUS
CN 2-Propanone (9CI) (CA INDEX NAME)



RN 75-07-0 HCAPLUS
CN Acetaldehyde (8CI, 9CI) (CA INDEX NAME)



RN 123-38-6 HCAPLUS
CN Propanal (9CI) (CA INDEX NAME)

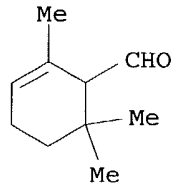


IT **432-24-6**, α-Cyclocitral **432-25-7** **41793-01-5**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**

(allylation of, by allyl bromide)

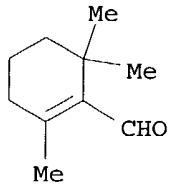
RN 432-24-6 HCAPLUS

CN 2-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



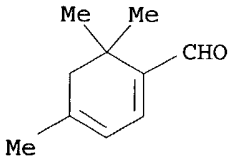
RN 432-25-7 HCAPLUS

CN 1-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 41793-01-5 HCAPLUS

CN 1,3-Cyclohexadiene-1-carboxaldehyde, 4,6,6-trimethyl- (6CI, 9CI) (CA INDEX NAME)



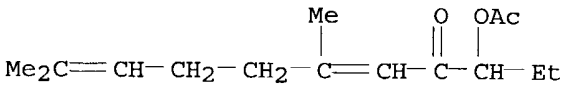
IT **127897-51-2P**

RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**

(preparation and cyclization of)

RN 127897-51-2 HCAPLUS

CN 5,9-Undecadien-4-one, 3-(acetyloxy)-6,10-dimethyl- (9CI) (CA INDEX NAME)

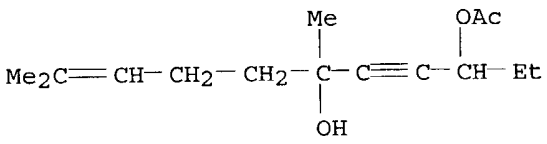


IT **127897-50-1P**

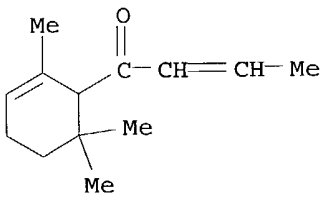
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**

(preparation and dehydrogenation-oxidation of)

RN 127897-50-1 HCAPLUS
CN 9-Undecen-4-yne-3,6-diol, 6,10-dimethyl-, 3-acetate (9CI) (CA INDEX NAME)

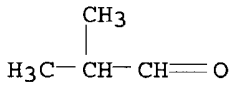


IT **43052-87-5P**, α-Damascone
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of, from α-cyclocitral)
RN 43052-87-5 HCAPLUS
CN 2-Buten-1-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)

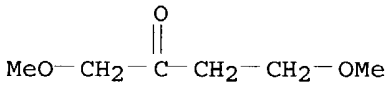


L43 ANSWER 9 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1983:160277 HCAPLUS
DOCUMENT NUMBER: 98:160277
TITLE: Chemistry of 2-methoxy-2,5-cyclohexadienones. I. Photochemistry of 2-methoxy-4,4-dimethyl-2,5-cyclohexadienone
AUTHOR(S): Matoba, Katsuhide; Karibe, Norio; Yamazaki, Takao
CORPORATE SOURCE: Fac. Pharm. Sci., Toyama Med. Pharm. Univ., Toyama, 930-01, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1982), 30(11), 3906-11
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Irradiation of the title compound (I) in MeOH gave 36.5% bicyclohexanone II and 7.8% cyclohexenone III, whereas irradiation of I in MeOH containing **catalytic** H2SO4 gave 35.4% cyclopentenone IV.
CC 24-7 (Alicyclic Compounds)
IT **78-84-2**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(cyclocondensation of, with dimethoxybutanone, cyclohexane from)
IT **25680-86-8**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(cyclocondensation of, with isobutylaldehyde, cyclohexane from)
IT **1074-26-6**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(methanolysis of)
IT **42117-30-6**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(photochem. of)

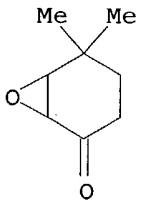
IT **42117-32-8P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and oxidation of)
IT 1128-57-0P 82700-85-4P **85312-28-3P** 85312-29-4P 85312-30-7P 85312-31-8P 85312-32-9P 85312-33-0P 85312-34-1P 85312-35-2P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
IT **78-84-2**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(cyclocondensation of, with dimethoxybutanone, cyclohexane from)
RN 78-84-2 HCAPLUS
CN Propanal, 2-methyl- (9CI) (CA INDEX NAME)



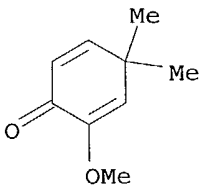
IT **25680-86-8**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(cyclocondensation of, with isobutylaldehyde, cyclohexane from)
RN 25680-86-8 HCAPLUS
CN 2-Butanone, 1,4-dimethoxy- (6CI, 8CI, 9CI) (CA INDEX NAME)



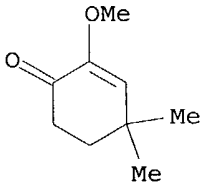
IT **1074-26-6**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(methanolysis of)
RN 1074-26-6 HCAPLUS
CN 7-Oxabicyclo[4.1.0]heptan-2-one, 5,5-dimethyl- (8CI, 9CI) (CA INDEX NAME)



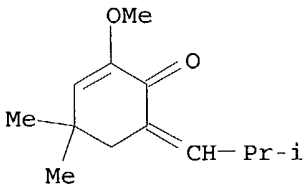
IT **42117-30-6**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(photochem. of)
RN 42117-30-6 HCAPLUS
CN 2,5-Cyclohexadien-1-one, 2-methoxy-4,4-dimethyl- (9CI) (CA INDEX NAME)



IT **42117-32-8P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and oxidation of)
RN 42117-32-8 HCAPLUS
CN 2-Cyclohexen-1-one, 2-methoxy-4,4-dimethyl- (9CI) (CA INDEX NAME)



IT **85312-28-3P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
RN 85312-28-3 HCAPLUS
CN 2-Cyclohexen-1-one, 2-methoxy-4,4-dimethyl-6-(2-methylpropylidene)- (9CI) (CA INDEX NAME)



L43 ANSWER 10 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:	1982:19758 HCAPLUS
DOCUMENT NUMBER:	96:19758
TITLE:	An improved two-step route for the preparation of β-diketones from aldehydes and its application to the synthesis of β-damascone
AUTHOR(S):	Pellicciari, Roberto; Fringuelli, Renata; Sisani, Ettore; Curini, Massimo
CORPORATE SOURCE:	Ist. Chim. Farm. Tossicol., Univ. Studi, Perugia, Italy
SOURCE:	Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1981), (9), 2566-9 CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE:	Journal

LANGUAGE: English

AB α-Diazo-β-hydroxyketones, prepared by the condensation reaction of aldehydes with MeCOC(Li):N2 (I), gave the corresponding β-diketones when exposed to Rh2(OAc)4. E.g., PhCH2CHO condensed with I [THF, (Me2CH)2NH, -78°, 30 min] to give 61% PhCH2CH(OH)C(:N2)COMe, which gave 77% PhCH2COCH2COMe with Rh2(OAc)4 **catalyst** [MeO(CH2)2OMe, 2 min]. The usefulness of the reaction is shown in the preparation of the terpenoid β-damascone (II; R = (E)-COCH:CHMe) (III). II [R = CH(OH)C(:N2)COMe], prepared from II (R = CHO) and I, gave 86% II (R = COCH:CMeOH) with Rh2(OAc)4 (MeOCH2CH2OMe, 3 h), which on treatment with oxalyl chloride followed by dehalogenation (Ag-Zn couple) gave III.

CC 25-16 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 24, 30

ST hydroxyketone diazo prepn elimination; ketone diazo hydroxy; diazohydroxyketone prepn diazo elimination; diketone beta; terpene damascone total synthesis; diazo elimination diazohydroxyketone rhodium **catalyst**; condensation diazolithiumacetone aldehyde; diketone prepn diazohydroxyketone elimination

IT Elimination reaction **catalysts**
(rhodium(II) acetate, for diazohydroxyketones)

IT Ketones, reactions
(diazohydroxy-, elimination reaction of, diketones by rhodium-**catalyzed**)

IT 15956-28-2
RL: CAT (Catalyst use); USES (Uses)
(**catalysts**, for diazo elimination reaction of diazohydroxyketones)

IT **2684-62-0**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(condensation reaction of, with aldehydes, diazohydroxyketones by)

IT **122-78-1 123-72-8 432-25-7 947-91-1**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(condensation reaction of, with diazolithioacetone, diazohydroxyketone by)

IT **39910-61-7 55718-68-8**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(diazo elimination reaction of, diketone by rhodium-**catalyzed**)

IT **80253-72-1P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and chlorination of)

IT **77250-09-0P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and dechlorination of, damascone by)

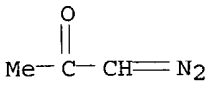
IT 77250-07-8P 80253-69-6P 80253-70-9P 80253-71-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and diazo elimination reaction of, rhodium(II) acetate-**catalyzed**)

IT 93-91-4P 3318-61-4P 7307-02-0P 15069-43-9P 24243-60-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by rhodium-**catalyzed** diazo elimination reaction of diazohydroxyketone)

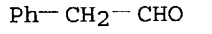
IT **23726-91-2P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(total synthesis of)

IT **2684-62-0**

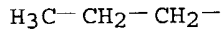
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(condensation reaction of, with aldehydes, diazohydroxyketones by)
RN 2684-62-0 HCAPLUS
CN 2-Propanone, 1-diazo- (8CI, 9CI) (CA INDEX NAME)



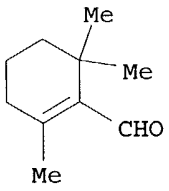
IT **122-78-1 123-72-8 432-25-7 947-91-1**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(condensation reaction of, with diazolithioacetone, diazohydroxyketone by)
RN 122-78-1 HCAPLUS
CN Benzeneacetaldehyde (9CI) (CA INDEX NAME)



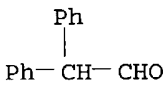
RN 123-72-8 HCAPLUS
CN Butanal (9CI) (CA INDEX NAME)



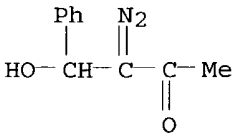
RN 432-25-7 HCAPLUS
CN 1-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



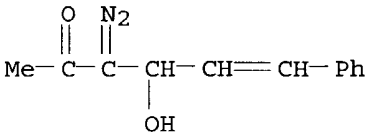
RN 947-91-1 HCAPLUS
CN Benzeneacetaldehyde, α-phenyl- (9CI) (CA INDEX NAME)



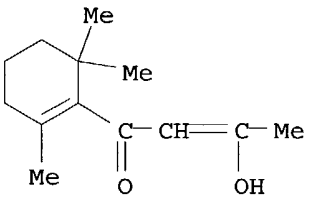
IT **39910-61-7 55718-68-8**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(diazo elimination reaction of, diketone by rhodium-**catalyzed**)
RN 39910-61-7 HCAPLUS
CN 2-Butanone, 3-diazo-4-hydroxy-4-phenyl- (9CI) (CA INDEX NAME)



RN 55718-68-8 HCAPLUS
CN 5-Hexen-2-one, 3-diazo-4-hydroxy-6-phenyl- (9CI) (CA INDEX NAME)

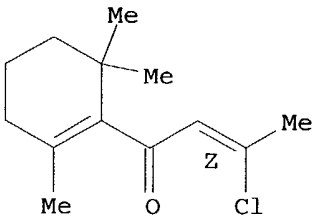


IT **80253-72-1P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and chlorination of)
RN 80253-72-1 HCAPLUS
CN 2-Buten-1-one, 3-hydroxy-1-(2,6,6-trimethyl-1-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



IT **77250-09-0P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and dechlorination of, damascone by)
RN 77250-09-0 HCAPLUS
CN 2-Buten-1-one, 3-chloro-1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (Z)- (9CI) (CA INDEX NAME)

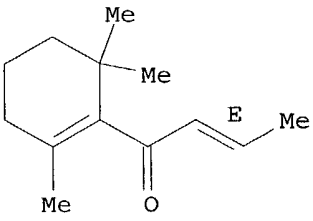
Double bond geometry as shown.



IT **23726-91-2P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**

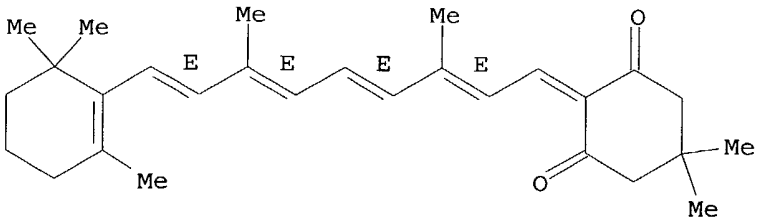
(total synthesis of)
RN 23726-91-2 HCAPLUS
CN 2-Buten-1-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



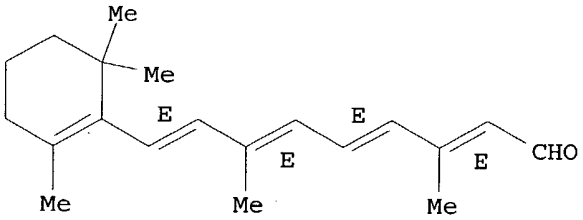
L43 ANSWER 11 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1980:461050 HCAPLUS
DOCUMENT NUMBER: 93:61050
TITLE: Potential prophylactic antitumor activity of retinylidene 1,3-diketones
AUTHOR(S): Acton, Nancy; Brossi, Arnold; Newton, Dianne L.; Sporn, Michael B.
CORPORATE SOURCE: Natl. Cancer Inst., Bethesda, MD, 20014, USA
SOURCE: Journal of Medicinal Chemistry (1980), 23(7), 805-9
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The title compds. were prepared by condensation of retinal [116-31-4] with acyclic-or cyclic diketones using piperidine and piperidine acetate as the **catalyst**. Cyclohexane-1,3-dione derivs. were the most active compds. in hamster tracheal organ culture assay to predict potential use for prevention of epithelial cancer. (all-E)-2-Retinylidene-5,5-dimethyl-1,3-cyclohexanedione (I) [70424-15-6] was selected for further evaluation.
CC 1-4 (Pharmacodynamics)
Section cross-reference(s): 25
IT 6991-16-8P 70359-68-1P 70359-69-2P **70424-15-6P** 73685-14-0P
73685-15-1P 73685-16-2P 73685-17-3P 73685-18-4P 73685-19-5P
73685-20-8P 73685-21-9P 73685-22-0P 73685-23-1P 73685-24-2P
73685-25-3P 73685-26-4P 73685-27-5P 73685-28-6P 73729-46-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation and neoplasm-inhibiting activity of)
IT **116-31-4**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(reaction of, with diketones)
IT **70424-15-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation and neoplasm-inhibiting activity of)
RN 70424-15-6 HCAPLUS
CN 1,3-Cyclohexanedione, 2-[(2E,4E,6E,8E)-3,7-dimethyl-9-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2,4,6,8-nonatetraenylidene]-5,5-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IT **116-31-4**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(reaction of, with diketones)
RN 116-31-4 HCAPLUS
CN Retinal (9CI) (CA INDEX NAME)

Double bond geometry as shown.



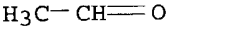
L43 ANSWER 12 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1980:75969 HCAPLUS
DOCUMENT NUMBER: 92:75969
TITLE: 1-Acyl-2,6,6-trimethylcyclohexene derivatives, intermediates and organoleptic uses
INVENTOR(S): Trenkle, Robert W.; Mookherjee, Braja D.; Kasper, Robin; Vock, Manfred H.; Vinals, Joaquin; Kiwala, Jacob; Schmitt, Frederick L.
PATENT ASSIGNEE(S): International Flavors and Fragrances Inc., USA
SOURCE: U.S., 33 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4172850	A	19791030	US 1978-965418	19781201
US 4196306	A	19800401	US 1979-39153	19790515
US 4209542	A	19800624	US 1979-39360	19790515
US 4210553	A	19800701	US 1979-39194	19790515
US 4215704	A	19800805	US 1979-39158	19790515
US 4217252	A	19800812	US 1979-39193	19790515

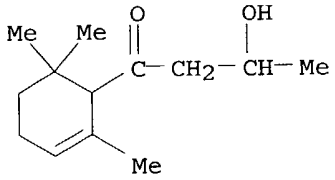
PRIORITY APPLN. INFO.: US 1978-965418 19781201
AB The hydrogenation of 1-acetyl-2,6,6-trimethyl-1,3-cyclohexadiene (I) over Pd/CaCO3 or Pd/BaSO4 at 0-100° and 1-100 atm gave

1-acetyl-2,6,6-trimethyl-2-cyclohexene (II), which demonstrated its usefulness in perfume compns. and as a flavoring material in food and tobacco. Thus, I in EtOAc containing quinoline was hydrogenated over Pd/BaSO4 at room temperature and 1 atm to give a mixture of II and 1-acetyl-2,6,6-trimethyl-1-cyclohexene.

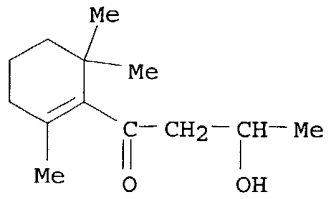
IC C07C045-00; C07B001-00
NCL 260586000P
CC 24-5 (Alicyclic Compounds)
Section cross-reference(s): 17, 62
IT **75-07-0**, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(addition reaction of, with acetylcyclohexenes and ethylmagnesium bromide)
IT 7440-05-3, uses and miscellaneous
RL: CAT (Catalyst use); USES (Uses)
(**catalysts**, for selective hydrogenation of acetylcyclohexadiene derivative)
IT **39900-15-7P 39900-16-8P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and dehydration of)
IT **35044-68-9P 43052-87-5P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
IT **41436-46-8**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(selective hydrogenation of)
IT **75-07-0**, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(addition reaction of, with acetylcyclohexenes and ethylmagnesium bromide)
RN 75-07-0 HCAPLUS
CN Acetaldehyde (8CI, 9CI) (CA INDEX NAME)



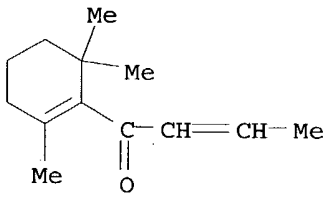
IT **39900-15-7P 39900-16-8P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and dehydration of)
RN 39900-15-7 HCAPLUS
CN 1-Butanone, 3-hydroxy-1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



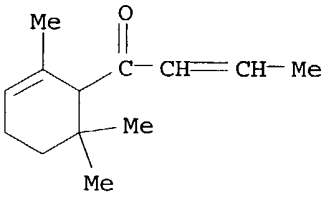
RN 39900-16-8 HCAPLUS
CN 1-Butanone, 3-hydroxy-1-(2,6,6-trimethyl-1-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



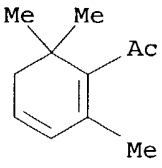
IT **35044-68-9P 43052-87-5P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
RN 35044-68-9 HCAPLUS
CN 2-Buten-1-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



RN 43052-87-5 HCAPLUS
CN 2-Buten-1-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



IT **41436-46-8**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(selective hydrogenation of)
RN 41436-46-8 HCAPLUS
CN Ethanone, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)- (9CI) (CA INDEX NAME)

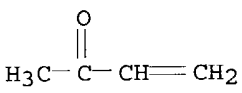


L43 ANSWER 13 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1979:523360 HCAPLUS
DOCUMENT NUMBER: 91:123360
TITLE: Michael-type addition of isobutyraldehyde to 1-buten-3-one **catalyzed** by tributylphosphine
AUTHOR(S): Miyakoshi, Tetsuo; Omichi, Hiroaki; Saito, Shojiro
CORPORATE SOURCE: Fac. Eng., Meiji Univ., Kawasaki, 214, Japan
SOURCE: Nippon Kagaku Kaishi (1979), (6), 748-53
CODEN: NKAKB8; ISSN: 0369-4577
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

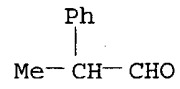
AB The reaction of Me2CHCHO (I) with CH2CHCOMe (II) **catalyzed** by Bu3P yielded 70% 2,2-dimethyl-5-oxohexanal. 4,4-Dimethyl-2-cyclohexen-1-one, 4,4-dimethyl-6-(2-methylpropylidene)-2-cyclohexen-1-one, and 3-hydroxy-4,4-dimethylcyclohexanone were also formed as by-products. The reaction of dialkylacetaldehydes with MVK yielded 2,2-dialkyl-5-oxohexanal. The reaction of I with other vinyl compds. such as acrylonitrile, 1-penten-3-one, and Me acrylate promoted by Bu3P was also examined Trioctylphosphine was also effective as a **catalyst** for the Michael type addition of I to II. The results indicate that the Michael type addition involves formation of a phosphonium betaine intermediate.

CC 23-15 (Aliphatic Compounds)
ST addn isobutyraldehyde butenone **catalyst**
IT Addition reaction **catalysts**
(tributylphosphine, for isobutyraldehyde with butenone)
IT **78-94-4**, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(addition reaction of, with aldehydes)
IT **93-53-8 96-17-3 97-96-1 123-05-7 123-15-9**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(addition reaction of, with butenone)
IT **96-33-3** 107-13-1, reactions **140-88-5**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(addition reaction of, with isobutyraldehyde)
IT **78-84-2**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(addition reaction of, with unsatd. compds.)
IT 998-40-3
RL: CAT (Catalyst use); USES (Uses)
(**catalysts**, for addition reaction of isobutyraldehyde with butenone and related compds.)
IT 1073-13-8P 4007-81-2P 5621-44-3P 6140-61-0P 13544-11-1P 70105-73-6P 70105-74-7P 70105-75-8P 70105-76-9P **71385-26-7P** 71385-27-8P 71385-28-9P 71385-29-0P 71385-30-3P 71385-31-4P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
IT **78-94-4**, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(addition reaction of, with aldehydes)
RN 78-94-4 HCAPLUS
CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)

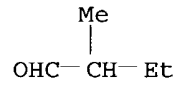


IT **93-53-8 96-17-3 97-96-1 123-05-7**

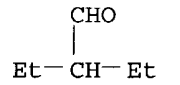
123-15-9
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(addition reaction of, with butenone)
RN 93-53-8 HCAPLUS
CN Benzeneacetaldehyde, α-methyl- (9CI) (CA INDEX NAME)



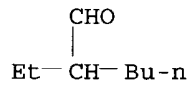
RN 96-17-3 HCAPLUS
CN Butanal, 2-methyl- (9CI) (CA INDEX NAME)



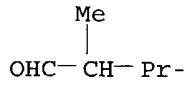
RN 97-96-1 HCAPLUS
CN Butanal, 2-ethyl- (9CI) (CA INDEX NAME)



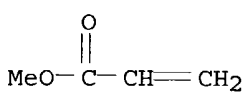
RN 123-05-7 HCAPLUS
CN Hexanal, 2-ethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



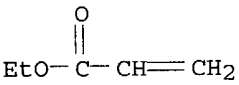
RN 123-15-9 HCAPLUS
CN Pentanal, 2-methyl- (9CI) (CA INDEX NAME)



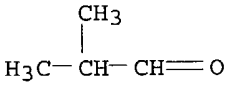
IT **96-33-3 140-88-5**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(addition reaction of, with isobutyraldehyde)
RN 96-33-3 HCAPLUS
CN 2-Propenoic acid, methyl ester (9CI) (CA INDEX NAME)



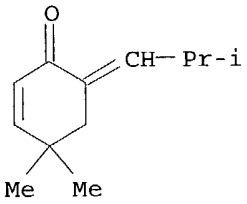
RN 140-88-5 HCAPLUS
CN 2-Propenoic acid, ethyl ester (9CI) (CA INDEX NAME)



IT **78-84-2**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(addition reaction of, with unsatd. compds.)
RN 78-84-2 HCAPLUS
CN Propanal, 2-methyl- (9CI) (CA INDEX NAME)



IT **71385-26-7P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
RN 71385-26-7 HCAPLUS
CN 2-Cyclohexen-1-one, 4,4-dimethyl-6-(2-methylpropylidene)- (9CI) (CA INDEX NAME)



L43 ANSWER 14 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1978:563788 HCAPLUS
DOCUMENT NUMBER: 89:163788
TITLE: Synthesis of α-damascone [trans-1-(2,6,6-trimethylcyclohex-2-enyl)but-2-en-1-one] by a **catalyzed** Diels-Alder reaction with inverse electron demand
AUTHOR(S): Cookson, Richard C.; Tuddenham, Robert M.
CORPORATE SOURCE: Chem. Dep., Univ. Southampton, Southampton, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1978), (6), 678-80
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Me2C:CH2 was added to a solution of cis- and trans-CH2:CHCMe:CHCOMe (20:80 mixture) and AlCl3 at room temperature (4 h) to give the five addition products I (R = Me, R1 = COMe; R = CH2COMe, R1 = H) II, III, and IV in the ratio 20:6:55:15:4. Sequential treatment of I (R = Me, R1 = COMe) with

PhNMeMgCl and MeCHO gave an aldol which dehydrated on treatment with NaOAc in Ac2O to give α-damascone (I; R = Me, R1 = COCH:CHMe).

CC 30-40 (Terpenoids)
Section cross-reference(s): 23

IT **20432-48-8 51905-49-8**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(Diels-Alder reaction of, with methylpropene)

IT **27539-94-2 27575-61-7**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(cyclization of)

IT **39900-15-7P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and dehydration of)

IT **37709-66-3P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and reaction of, with methylanilinomagnesium bromide and acetaldehyde)

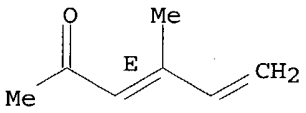
IT **24720-09-0P** 37709-65-2P 37709-71-0P 67927-75-7P 67927-76-8P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)

IT **75-07-0**, reactions
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(reaction of, with bromomethylaniline and acetyltrimethylcyclohexene)

IT **20432-48-8 51905-49-8**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(Diels-Alder reaction of, with methylpropene)

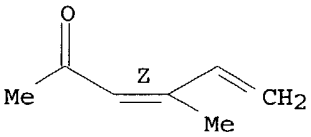
RN 20432-48-8 HCAPLUS
CN 3,5-Hexadien-2-one, 4-methyl-, (E)- (8CI, 9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 51905-49-8 HCAPLUS
CN 3,5-Hexadien-2-one, 4-methyl-, (Z)- (9CI) (CA INDEX NAME)

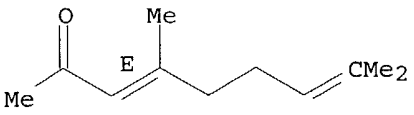
Double bond geometry as shown.



IT **27539-94-2 27575-61-7**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(cyclization of)

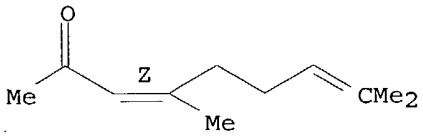
RN 27539-94-2 HCAPLUS
CN 3,7-Nonadien-2-one, 4,8-dimethyl-, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

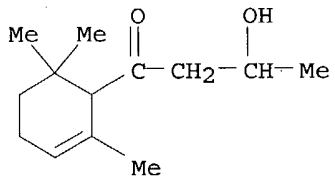


RN 27575-61-7 HCAPLUS
CN 3,7-Nonadien-2-one, 4,8-dimethyl-, (3Z)- (9CI) (CA INDEX NAME)

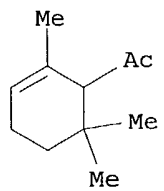
Double bond geometry as shown.



IT **39900-15-7P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and dehydration of)
RN 39900-15-7 HCAPLUS
CN 1-Butanone, 3-hydroxy-1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



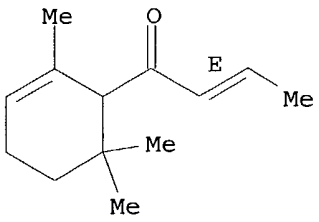
IT **37709-66-3P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and reaction of, with methylanilinomagnesium bromide and acetaldehyde)
RN 37709-66-3 HCAPLUS
CN Ethanone, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



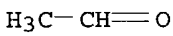
IT **24720-09-0P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
RN 24720-09-0 HCAPLUS

CN 2-Buten-1-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

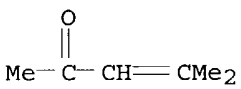


IT **75-07-0**, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(reaction of, with bromomethylaniline and acetyltrimethylcyclohexene)
RN 75-07-0 HCAPLUS
CN Acetaldehyde (8CI, 9CI) (CA INDEX NAME)

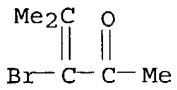


L43 ANSWER 15 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1975:606442 HCAPLUS
DOCUMENT NUMBER: 83:206442
TITLE: Synthesis of α-damascone [trans-1-(2,6,6-trimethylcyclohex-3-enyl)but-2-en-1-one] and β-damascenone [trans-1-(2,6,6-trimethylcyclohexa-1,3-dienyl)but-2-en-1-one]
AUTHOR(S): Ayyar, K. Subrahmania; Cookson, Richard C.; Kagi, Douglas A.
CORPORATE SOURCE: Chem. Dep., Univ. Southampton, Southampton, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1975), (17), 1727-36
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Diels-Alder addition of CH2:CHCH:CHMe to Me2C:CBrCOMe **catalyzed** by AlCl3 gave the cyclohexenes I (R = Me, R1 = H; R = H, R1 = Me) which on dehydrobromination gave 1-acetyl-2,6,6-trimethylcyclohexa-1,3-diene. Aldol condensation of the diene with MeCHO followed by dehydration of the resulting aldol gave β-damascenone II. CH2:CHCH:CHMe with Me2C:CHCOMe gave δ-damascone III by a similar route.
CC 30-15 (Terpenoids)
Section cross-reference(s): 11, 24
IT **141-79-7 5682-80-4 58031-23-5**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(Diels-Alder reaction with pentadiene)
IT **75-07-0**, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(aldol condensation reaction with acetyltrimethylcyclohexene)
IT **41436-09-3P 41436-45-7P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**

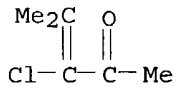
(preparation and dehydrobromination of)
IT **31824-00-7P 41436-43-5P** 41436-47-9P 41436-49-1P
41436-50-4P 41436-51-5P 58031-24-6P 58031-25-7P 58031-26-8P
58031-27-9P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
IT **23726-93-4P 57378-68-4P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(total synthesis of)
IT **141-79-7 5682-80-4 58031-23-5**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(Diels-Alder reaction with pentadiene)
RN 141-79-7 HCAPLUS
CN 3-Penten-2-one, 4-methyl- (8CI, 9CI) (CA INDEX NAME)



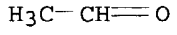
RN 5682-80-4 HCAPLUS
CN 3-Penten-2-one, 3-bromo-4-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 58031-23-5 HCAPLUS
CN 3-Penten-2-one, 3-chloro-4-methyl- (6CI, 9CI) (CA INDEX NAME)

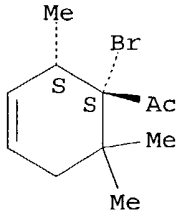


IT **75-07-0**, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(aldol condensation reaction with acetyltrimethylcyclohexene)
RN 75-07-0 HCAPLUS
CN Acetaldehyde (8CI, 9CI) (CA INDEX NAME)



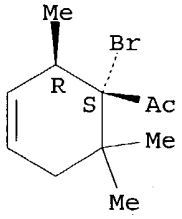
IT **41436-09-3P 41436-45-7P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP
(Preparation); **RACT (Reactant or reagent)**
(preparation and dehydrobromination of)
RN 41436-09-3 HCAPLUS
CN Ethanone, 1-(1-bromo-2,6,6-trimethyl-3-cyclohexen-1-yl)-, cis- (9CI) (CA
INDEX NAME)

Relative stereochemistry.



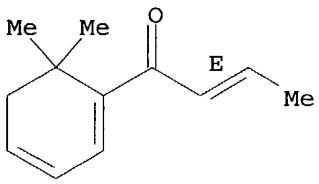
RN 41436-45-7 HCAPLUS
CN Ethanone, 1-(1-bromo-2,6,6-trimethyl-3-cyclohexen-1-yl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



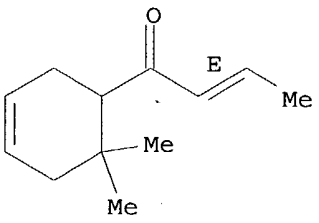
IT **31824-00-7P 41436-43-5P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
RN 31824-00-7 HCAPLUS
CN 2-Buten-1-one, 1-(6,6-dimethyl-1,3-cyclohexadien-1-yl)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



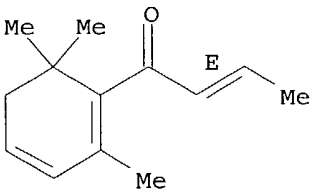
RN 41436-43-5 HCAPLUS
CN 2-Buten-1-one, 1-(6,6-dimethyl-3-cyclohexen-1-yl)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

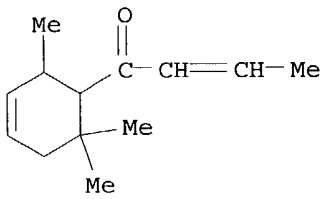


IT **23726-93-4P 57378-68-4P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(total synthesis of)
RN 23726-93-4 HCAPLUS
CN 2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (2E)- (9CI)
(CA INDEX NAME)

Double bond geometry as shown.



RN 57378-68-4 HCAPLUS
CN 2-Buten-1-one, 1-(2,6,6-trimethyl-3-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



L43 ANSWER 16 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1975:592676 HCAPLUS
DOCUMENT NUMBER: 83:192676
TITLE: 2,6,6-Trimethyl-1-crotonoyl-2-cyclohexene
INVENTOR(S): Takagi, Yoshikazu; Kogami, Kunio; Hayashi, Kazuo
PATENT ASSIGNEE(S): Hasegawa, T., Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 50069047	A2	19750609	JP 1973-117803	19731022

PRIORITY APPLN. INFO.: JP 1973-117803 19731022

AB The title compound (I) was prepared by addition reaction of II with an allylmagnesium halide or allyllithium, followed by hydrolysis to give III, which was oxidized to give IV, followed by acid- or alkali-**catalyzed** isomerization. I, III, and IV are useful as perfumes. Thus, 38.0 g II in 100 ml anhydrous Et2O was added in 2 hr at 0-5° to CH2:CHCH2MgBr, the mixture reacted 3 hr at 20-25° and poured into 500 ml saturated aqueous NH4Cl to give 92% III. A solution of CrO3 20.0 in H2SO4 30.0 and H2O 150 g was added in 2 hr at 5-10° to a solution of 48.5 g III

in 300 ml Me2CO and the mixture reacted 2 hr at 10-15° to give 94% IV. P-MeC6H4SO3H (1.2 g) was added to a solution of 24.0 g IV in 300 ml C6H6 and the mixture refluxed 2 hr at 78-80° to give 98% I.

NCL 16C852

CC 24-5 (Alicyclic Compounds)
Section cross-reference(s): 62, 30

IT **432-24-6**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(Grignard reaction of, with allyl bromide)

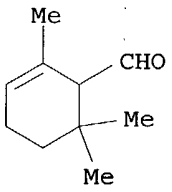
IT **31089-90-4P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and rearrangement of)

IT **43052-87-5P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)

IT **432-24-6**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(Grignard reaction of, with allyl bromide)

RN 432-24-6 HCAPLUS

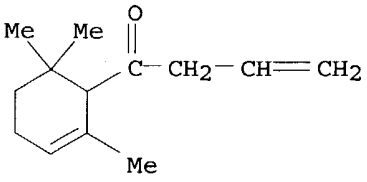
CN 2-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **31089-90-4P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and rearrangement of)

RN 31089-90-4 HCAPLUS

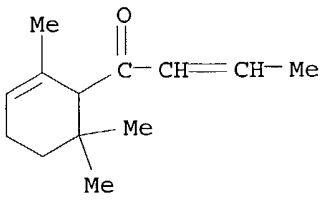
CN 3-Buten-1-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- (8CI, 9CI) (CA INDEX NAME)



IT **43052-87-5P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)

RN 43052-87-5 HCAPLUS

CN 2-Buten-1-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



L43 ANSWER 17 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1974:520815 HCAPLUS
DOCUMENT NUMBER: 81:120815
TITLE: Regiospecific acylation, alkylation, and aldol condensation using magnesium enolates resulting from the conjugate addition of Grignard reagents to α,β-unsaturated ketones
AUTHOR(S): Naef, Ferdinand; Decorzant, Rene
CORPORATE SOURCE: Res. Lab., Firmenich S. A., Geneva, Switz.
SOURCE: Helvetica Chimica Acta (1974), 57(5), 1317-27
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Mg 3,3-dimethyl-1-cyclohexenolate (I), formed in Cu-**catalyzed** addition of MeMgI to 3-methyl-2-cyclohexen-1-one, was subjected toregiospecific reactions (acylation, alkylation, aldol condensation, etc.) in order to find a new access to the damascones, ionones, and carotenoids. Thus, cyclohexanone II (Z = O, R = COMe), obtained from reaction of I with AcCl, was treated with MeMgI to give II (Z = OH, Me; R = COMe), which was dehydrated to II (Z = CH2, R = COMe). The latter was condensed with MeCHO in the presence of PhNMeMgBr to give γ-damascone (II, Z = CH2, R = COCH:CHMe).

CC 30-40 (Terpenoids)

IT 1197-92-8P 2979-19-3P 37709-66-3P 54200-56-5P 54200-57-6P
54200-59-8P 54200-60-1P 54200-61-2P **54200-62-3P**
54200-63-4P 54200-64-5P 54201-07-9P 54201-08-0P 54201-09-1P
54201-10-4P 57074-03-0P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)

IT **75-36-5** 106-95-6 107-05-1 926-57-8 **4170-30-3**
5392-40-5 10487-71-5 54201-06-8
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(reaction of, with magnesium 3,3-dimethyl-1-cyclohexenolate)

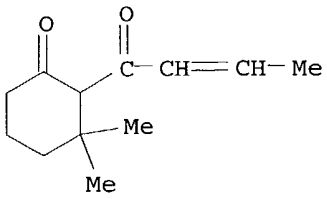
IT **1193-18-6**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(reaction of, with methyl magnesium iodide)

IT **35087-49-1**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(synethesis of)

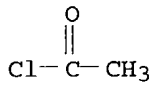
IT **75-07-0**, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(with magnesium 3,3-dimethyl-1-cyclohexenolate)

IT **54200-62-3P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)

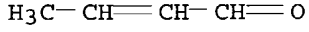
RN 54200-62-3 HCAPLUS
CN Cyclohexanone, 3,3-dimethyl-2-(1-oxo-2-butenyl)- (9CI) (CA INDEX NAME)



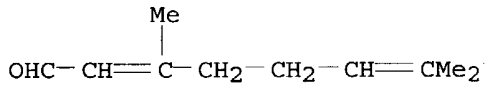
IT **75-36-5 4170-30-3 5392-40-5 10487-71-5**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(reaction of, with magnesium 3,3-dimethyl-1-cyclohexenolate)
RN 75-36-5 HCAPLUS
CN Acetyl chloride (8CI, 9CI) (CA INDEX NAME)



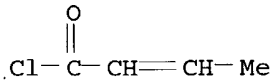
RN 4170-30-3 HCAPLUS
CN 2-Butenal (9CI) (CA INDEX NAME)



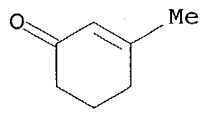
RN 5392-40-5 HCAPLUS
CN 2,6-Octadienal, 3,7-dimethyl- (8CI, 9CI) (CA INDEX NAME)



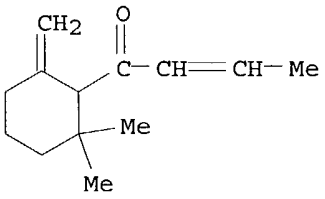
RN 10487-71-5 HCAPLUS
CN 2-Butenoyl chloride (9CI) (CA INDEX NAME)



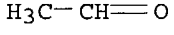
IT **1193-18-6**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(reaction of, with methyl magnesium iodide)
RN 1193-18-6 HCAPLUS
CN 2-Cyclohexen-1-one, 3-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



IT **35087-49-1**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(synethesis of)
RN 35087-49-1 HCAPLUS
CN 2-Buten-1-one, 1-(2,2-dimethyl-6-methylenecyclohexyl)- (9CI) (CA INDEX NAME)



IT **75-07-0**, reactions
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(with magnesium 3,3-dimethyl-1-cyclohexenolate)
RN 75-07-0 HCAPLUS
CN Acetaldehyde (8CI, 9CI) (CA INDEX NAME)



L43 ANSWER 18 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1973:504808 HCAPLUS
DOCUMENT NUMBER: 79:104808
TITLE: 1-Cyclohexenyl alkenyl ketones
INVENTOR(S): Kovats, Ervin; Ohloff, Guenther; Demole, Edouard; Stoll, Max
PATENT ASSIGNEE(S): Firmenich S. A.
SOURCE: Patentschrift (Switz.), 4 pp.
CODEN: SWXXAS
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 537352	A	19730713	CH 1971-11593	19690808

PRIORITY APPLN. INFO.: CH 1971-11593 19690808

AB Allyl cyclohexenyl ketones (I; R = H, Me) are isomerized by p-MeC6H4SO3H to give the resp. 1-alkenyl cyclohexenyl ketones (II). I are prepared by oxidation of the corresponding carbinols.
IC C07C
CC 24-5 (Alicyclic Compounds)
Section cross-reference(s): 23
IT Isomerization **catalysts**
(toluenesulfonic acid, for allyl cyclohexenyl ketones, 1-alkenyl cyclohexenyl ketones from)
IT **432-25-7**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(allyl(trimethylcyclohexenyl)carbinol from)
IT 104-15-4, uses and miscellaneous

RL: CAT (Catalyst use); USES (Uses)
(**catalysts**, for isomerization of allyl cyclohexenyl ketones)

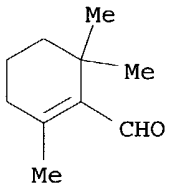
IT **79-76-5**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(epoxidn. of)

IT **31089-73-3 31204-29-2**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(isomerization of, **catalysts** for)

IT 31089-96-0P 31162-57-9P **31191-92-1P 31191-93-2P**
35044-68-9P 35896-31-2P 35896-32-3P 42741-51-5P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)

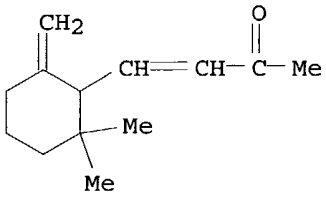
IT **432-25-7**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(allyl(trimethylcyclohexenyl)carbinol from)

RN 432-25-7 HCAPLUS
CN 1-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



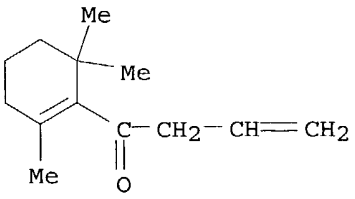
IT **79-76-5**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(epoxidn. of)

RN 79-76-5 HCAPLUS
CN 3-Buten-2-one, 4-(2,2-dimethyl-6-methylenecyclohexyl)- (7CI, 8CI, 9CI) (CA INDEX NAME)

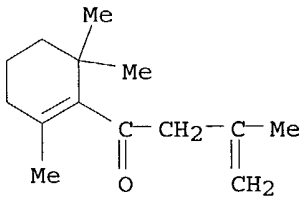


IT **31089-73-3 31204-29-2**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(isomerization of, **catalysts** for)

RN 31089-73-3 HCAPLUS
CN 3-Buten-1-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)- (8CI, 9CI) (CA INDEX NAME)

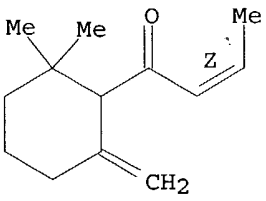


RN 31204-29-2 HCAPLUS
CN 3-Buten-1-one, 3-methyl-1-(2,6,6-trimethyl-1-cyclohexen-1-yl)- (8CI, 9CI) (CA INDEX NAME)



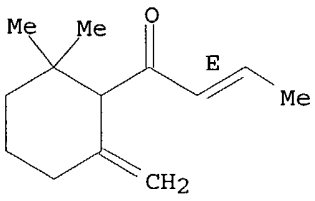
IT **31191-92-1P 31191-93-2P 35044-68-9P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
RN 31191-92-1 HCAPLUS
CN 2-Buten-1-one, 1-(2,2-dimethyl-6-methylenecyclohexyl)-, (Z)- (8CI, 9CI) (CA INDEX NAME)

Double bond geometry as shown.

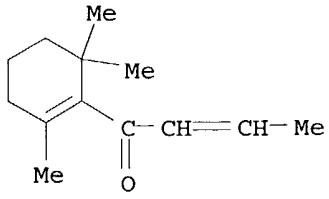


RN 31191-93-2 HCAPLUS
CN 2-Buten-1-one, 1-(2,2-dimethyl-6-methylenecyclohexyl)-, (E)- (8CI, 9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 35044-68-9 HCAPLUS
CN 2-Buten-1-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)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